International Materials Reviews

ISSN: 0950-6608 (Print) 1743-2804 (Online) Journal homepage: https://www.tandfonline.com/loi/yimr20

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To cite this article: Shuozhi Xu & Xiang Chen (2019) Modeling dislocations and heat conduction in crystalline materials: atomistic/continuum coupling approaches, International Materials Reviews, 64:7, 407-438, DOI: 10.1080/09506608.2018.1486358

To link to this article: https://doi.org/10.1080/09506608.2018.1486358

Published online: 25 Jun 2018.

INTERNATIONAL MATERIALS REVIEWS
2019, VOL. 64, NO. 7, 407–438
https://doi.org/10.1080/09506608.2018.1486358

FULL CRITICAL REVIEW

Modeling dislocations and heat conduction in crystalline materials: atomistic/continuum coupling approaches

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ABSTRACT

Dislocations and heat conduction are essential components that influence properties and performance of crystalline materials, yet the modelling of which remains challenging partly due to their multiscale nature that necessitates simultaneously resolving the short-range dislocation core, the long-range dislocation elastic field, and the transport of heat carriers such as phonons with a wide range of characteristic length scale. In this context, multiscale materials modelling based on atomistic/continuum coupling has attracted increased attention within the materials science community. In this paper, we review key characteristics of five representative atomistic/continuum coupling approaches, including the atomistic-to-continuum method, the bridging domain method, the concurrent atomistic–continuum method, the coupled atomistic/discrete-dislocation method, and the quasicontinuum method, as well as their applications to dislocations, heat conduction, and dislocation/phonon interactions in crystalline materials. Through problem-centric comparisons, we shed light on the advantages and limitations of each method, as well as the path towards enabling them to effectively model various material problems in engineering from nano- to mesoscale.

Abbreviations: AtC: atomistic-to-continuum; BCC: body-centred cubic; BDM: bridging domain method; CAC: concurrent atomistic–continuum; CADD: coupled atomistic/discrete-dislocation; DDD: discrete dislocation dynamics; DDf-MD: discrete diffusion-molecular dynamics; DOF: degree of freedom; ESCM: embedded statistical coupling method; FCC: face-centred cubic; GB: grain boundary; XFEM: extended finite element method; MD: molecular dynamics; MS: molecular statics; PK: Peach-Koehler; QC: quasicontinuum

ARTICLE HISTORY
Received 30 January 2018
Accepted 4 June 2018

KEYWORDS
Atomistic/continuum coupling; multiscale materials modelling; dislocations; heat conduction; phonon; dislocation/phonon interactions; finite temperature; crystalline materials

Introduction

Multiscale materials modelling methods can be categorised in terms of sequential and concurrent methods [1]. Sequential multiscale methods are approaches whereby simulations are first conducted at fine scale, the results of which are then processed to provide inputs to coarse-scale simulations [2]; it follows that the fine-scale model is no longer required. Atomistic simulation methods, for example, can be viewed as sequential multiscale approaches, since the interatomic potentials are usually informed by lower scale *ab initio* simulations.

Concurrent multiscale methods, as the name suggests, employ models at two or more length scales simultaneously [3]. Depending on whether the physical problem is decomposed into different regions, concurrent methods are further classified into two sub-categories: hierarchical and domain decomposition (also called partitioned-domain) methods. Hierarchical methods make use of all length scales everywhere, i.e. with the coarse-scale model making regular appeals to the fine-scale model to determine a constitutive law and, conversely, the fine-scale model looking to the coarse-scale model for its boundary conditions [1]. Domain decomposition methods, on the other hand, divide the problem into different contiguous, largely non-overlapping domains, all of which are updated concurrently in time. In most atomistic/continuum coupling domain decomposition methods, atomistic domains, in which atoms are updated in the same way as in atomistic methods such as molecular dynamics (MD) and molecular statics (MS), are employed where explicit descriptions of nanoscale structures and phenomena are essential [4]; otherwise, continuum domains are employed in various ways to reduce computational cost [1]. In the last 15 years, a plethora of reviews have been dedicated to analysing and comparing the theoretical foundations of different multiscale models [5–12]. For example, 14 atomistic/continuum coupling techniques were implemented in 2009 by Miller and Tadmor [13] to simulate a Lomer dislocation dipole for which the theories, numerical accuracy, and efficiency of these methods are compared. However, there is a lack of problem-centric comparison among different

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methods. As the multiscale modelling community is shifting its focus from method development to engineering application [14], it is imperative to review this emerging trend by comparing different methods in modelling the same material problems and to shed light on the path towards enabling multiscale modelling to make a real contribution to new materials science knowledge.

In this paper, we review multiscale modelling of dislocations and heat conduction in crystalline materials using atomistic/continuum coupling approaches. We remark that most concurrent multiscale methods, with some exceptions [15–18], are only applicable to crystalline materials because their atomic-level structures facilitate the atomistic/continuum coupling [12]. We purposely choose dislocations, either the Volterra dislocation (1D linear defect) or the extended dislocation (2D planar defect), in part because of their typicalities in representing a wide range of lattice defects. In a continuum, an extended dislocation is a weak discontinuity while a Volterra dislocation is a strong discontinuity [19]. Other strong discontinuities include a crack, whose propagation simulated using different atomistic/continuum coupling methods has been compared [20]. Besides the dislocation, we will also review heat conduction, with a focus on phonon-mediated heat conduction in crystalline materials. The capability of a method to solve the time-dependent heat conduction problem distinguishes it fundamentally from a static method; in addition, the way a method solves this problem, i.e. whether or not to employ empirical laws such as Fourier's law of heat conduction, marks the predictive power of the particular approach. We emphasise that it is not our intention to exhaustively review all multiscale atomistic/continuum coupling techniques in modelling dislocations and heat conduction; rather, we assess and compare five typical methods that have been actively developed in recent years, including the atomistic-to-continuum (AtC) method [21], the bridging domain method (BDM) [22], the concurrent atomistic–continuum (CAC) method [23], the coupled atomistic/discrete-dislocation (CADD) method [24], and the quasicontinuum (QC) method [25].

The paper is structured as follows. In the section 'Atomistic/continuum coupling', we discuss strengths, limitations, and outstanding challenges among atomistic/continuum coupling methods, before reviewing key characteristics of the five multiscale methods in the next section. Then, applications of BDM, CAC, and CADD to dislocations, those of AtC, BDM, CAC, and QC to heat conduction, as well as those of CAC to dislocation/phonon interactions are discussed in the three sections after next. In the end, conclusions, challenges, and perspectives are presented in the last two sections.

Atomistic/continuum coupling

Strengths and limitations

Over the past few decades, atomistic modelling has offered a powerful tool for gaining substantial insights into dislocations and heat conduction in crystalline materials. However, atomic-level simulations are limited to nano/submicron length scale even with dedicated high-performance computing resources; direct atomistic simulations of materials are usually conducted in simulation cells smaller than $(250\,\text{nm})^3$ with fewer than 1 billion atoms. On the other hand, classical continuum models do not naturally incorporate the discrete atomic-scale degrees of freedom (DOFs) and other evolving internal state variables associated with defects and heat [26–28]. Since its inception in the early 1990s [29], numerous atomistic/continuum coupling approaches have been developed to combine the atomistic domain (for describing short-range dislocation core and short-wavelength phonons) with the continuum domain (for addressing long-range dislocation elastic fields and long-wavelength phonons). By employing coarse-grained or reduced order models in regions away from those requiring short-range accuracy, these methods aim at simulating problems at scales that are not accessible to typical fully resolved atomistics. For the same material problem, a multiscale model contains much fewer DOFs than its atomistic counterpart; with the same computing power, using a multiscale method allows for accessing larger scale phenomena and conducting more parametric studies.

Most atomistic/continuum coupling methods share some algorithmic similarities with atomistic modelling techniques, especially in the atomistic domain [1]. For example, pressure/stress control in both atomistic and continuum domains can be realised by barostats such as volume rescaling, Andersen barostat [30], Berendsen barostat [31], and Parrinello-Rahman barostat [32]. Energy minimisation in static simulations and equations of motion in dynamic simulations can be implemented using well-established numerical schemes, e.g. conjugate gradient and velocity Verlet algorithms [1], respectively. Common parallel algorithms employed in atomistic simulations, including spatial decomposition, force decomposition, and atom decomposition [33], can be readily applied to both atomistic and continuum domains, with special attention paid to the issues arising from the potentially unequal processor workload in different domains and the geometric differences between the finite elements and the processor domains [34,35]. In terms of the dimensionality, similar to atomistics, many multiscale methods start with 1D or 2D formulations/applications for method validation, yet there is usually no theoretical challenge in extending them to tackle fully 3D problems.

Nevertheless, issues that plague atomistics, such as the uncertainty in the interatomic potential and the high strain rates in MD, remain in atomistic/continuum coupling approaches. Apart from the continuum domain itself, another source of error is the atomistic/continuum domain interface, across which there exists a change in material description, governing equations, and/or numerical resolution. Except in a few special cases, e.g. undeformed and affinely deformed configurations, a bi-material interface is effectively introduced, leading to numerical errors that may have non-negligible effects on the areas of interests in a simulation [13]. Thus, a key challenge arises from the necessity to losslessly and unimpededly exchange information (e.g. defects and heat) between the two domains, particularly from the atomistic to the continuum domain, because the reverse information flow is relatively more fluent owing to the more DOFs in atomistics [14]. For this reason, much effort has been devoted to improving information transmission from the atomistic domain to the continuum domain, particularly to addressing certain challenges that are common to domain decomposition methods. In the next three subsections, we discuss three outstanding challenges – atomistic/continuum coupling in static and dynamic settings, as well as mesh refinement – which play an important role in dislocations, heat conduction, and dislocation/phonon interactions.

Statics

The coupling between the atomistic and continuum domains for static problems comes in multiple forms, distinguished in four primary ways, including the governing formulation, the coupling boundary conditions, the handshake region, and the treatment of the continuum [1]. A summary of all five atomistic/continuum coupling methods reviewed here in the context of the four categories has been presented in the literature [13], except CAC, which employs a force-based governing formulation, a strong compatibility across the domain interface, no handshake region, and discontinuous finite elements in the continuum to admit certain linear and planar defects (e.g. dislocations, intrinsic stacking faults). We remark that any errors present in the static implementation will remain, if are not amplified, in the dynamic setting, which introduces new challenges to be discussed in the next subsection. For example, in terms of the governing formulation, the energy-based methods are built onminimising a well-defined energy functional for static problems [12]. However, they are inevitably accompanied by non-physical 'ghost forces' stemming from the combination of two energy functionals from different models, e.g. a local continuum model and a non-local atomistic model. In practice, the effects of the 'ghost forces' can be minimised in two ways: (i) calculating the 'ghost forces' in an undeformed model and subtracting them from the total forces in deformed models [36] and (ii) employing a non-local continuum model, e.g. in non-local QC [37] and CAC methods. Even in the absence of the 'ghost forces', from the perspective of the fidelity of the information flow, while the continuum domain in static setting can be tailored to fit a perfect crystalline material *a priori*, it is impeded from receiving all information associated with the 'disordered' atomic positions owing to potential nucleation and migration of lattice defects which may be present in the atomistic domain.

Finite temperature and dynamics

Most atomistic/continuum coupling methods have a static formulation for simulations effectively at 0 K, as well as a zero temperature dynamic formulation for simulations at near 0 K, the latter of which can be realised by damped dynamics or quenched dynamics [38]. We consider the static and zero temperature dynamic formulations a necessary condition for the recognition of any new atomistic/continuum coupling method. In practice, these two types of formulations enable a wide range of useful ideal applications from the scientific point of view. However, engineering materials usually serve at room/elevated temperatures, where atoms oscillate around an averaged configuration [39], the modelling of which requires equilibrium and non-equilibrium finite temperature dynamic formulations in both atomistic and continuum domains in a consistent manner. Here, non-equilibrium dynamics refers to physical systems that are not in thermodynamic equilibrium [40,41], i.e. there exist net macroscopic flows of matter or energy within a system or between systems, e.g. in heat conduction, diffusion, and fluid flow. In the continuum domain, in equilibrium dynamics, the average atomic configuration and associated mechanical quantities, including elastic constants, Poisson's ratio, and lattice defects properties (e.g. dislocation mobility and core disregistry/stress/energy, point defect formation/migration energy), may vary as a predefined function of the temperature; also, the temperature may be defined based entirely on the configurational but not kinetic information [42,43]. However, in non-equilibrium dynamics, the thermal fluctuation, which becomes increasingly pronounced in influencing material properties at higher temperatures, is difficult to attain [44,45].

In dynamic setting, different time steps may be employed in atomistic and continuum domains, e.g. in BDM [46], CADD [47], and the embedded statistical coupling method (ESCM) [48]. Otherwise, a uniform time step in an atomistic/continuum coupling method is governed by the smallest among all domains which is usually on the femtosecond scale because of the high

atomic-vibration frequency in the atomistic domain. Consequently, like *classical* MD, *classical* dynamic atomistic/continuum coupling methods are limited in their abilities to examine phenomena that occur over large timespans that may involve a combination of displacive and diffusive mechanisms [39,49]. The small timestep in MD also leads to an overdriven dynamics such that some local minima and saddle points on the potential energy surface are not accessed [50]. To this end, accelerated MD methods such as hyperdynamics [51], parallel replica dynamics [52], and temperature accelerated dynamics [53], as well as other methods coarse-graining in time (e.g. phase field crystal [54], diffusive MD [55], and long-time scale kinetic Monte Carlo [56]), can be utilised in the atomistic domain – sometimes in the continuum domain as well, e.g. in hyper-QC [57]– to extend the accessible time scale to several orders of magnitude larger than that in classical MD to simulate rare events such as cross-slip and diffusion [58].

Besides the aforementioned issues in static setting, there exist three unique challenges in formulating finite temperature dynamic atomistic/continuum coupling approaches:

- *Definition of temperature.* The temperature of a system in thermal equilibrium is a macroscopic property describing whether or not the system will exchange heat with another when the two are brought into thermal contact; the existence of an optimum temperature measurement in a non-equilibrium system is still a matter of debate and research [40]. In thermal equilibrium, the temperature T of a set of particles is usually defined as

$$T = \frac{2E_{\text{kin}}}{N_{\text{dim}} N_{\text{p}} k_{\text{B}}}, \tag{1}$$

  where k_{B} is the Boltzmann constant, N_{dim} is the dimensionality of the simulation, E_{kin} and N_{p} are, respectively, the total kinetic energy and the total number of particles in the system, including slave atoms which do not have independent DOFs. In the atomistic domain,

$$E_{\text{kin}} = \sum_{k}^{N_{\text{atom}}} \frac{1}{2} m_k \left|\dot{\mathbf{R}}_k\right|^2, \tag{2}$$

  where N_{atom} is the total number of atoms, m_k and $\dot{\mathbf{R}}_k$ are the mass and the velocity vector of the kth atom, respectively. In the continuum domain, without loss of generality, we assume that the nodes ξ are the only DOFs within an element, while positions of slave atoms/material points k are interpolated from the nodes. It follows that quantities of real atoms in the atomistic domain are replaced with those of nodes and slave atoms/material points within elements, i.e.

$$\begin{aligned} E_{\text{kin}} &= \sum_{I}^{N_{\text{ele}}} E_I^{\text{ele}} \\ &= \sum_{I}^{N_{\text{ele}}} \frac{1}{2} \left[\sum_{\xi}^{N_{\text{npe}}} m_\xi \left|\dot{\mathbf{R}}_\xi\right|^2 + \sum_{k}^{N_{\text{ape}}} m_k \left|\dot{\mathbf{R}}_k\right|^2 \right], \end{aligned} \tag{3}$$

  where E_I^{ele} is the kinetic energy of the Ith element, N_{ele} is the total number of finite elements in the continuum domain, N_{npe} and N_{ape} are the numbers of nodes and slave atoms/material points per element, respectively. Given the constrained status of the slave atoms/material points, it is not clear how their velocities should be calculated to yield an accurate prediction of E_{kin}. In practice, one simple and commonly adopted approach is to interpolate velocities of slave atoms/material points from the nodes, e.g. in a modified QC method [59]. However, this formulation does not take into account the entropic contribution from the thermal fluctuations of the constrained atoms/material points within elements [60]. While the missing entropy may be computed and added to Equation (3) by introducing local harmonic [61] or quasi-harmonic approximation [62], the continuum domain still cannot reproduce the exact kinetics as the atomistic domain, which may be further complicated if a handshake region is employed at the atomistic/continuum domain interface [63]. Moreover, in the atomistic domain, the temperature can be tuned about a desired value using the same thermostat, e.g. velocity rescaling, Andersen thermostat [30], Berendsen thermostat [31], and Nosé–Hoover thermostat [64–66]. However, it is questionable to use the particle-based thermostat to control the temperature in a continuum. To this end, separate temperature controls in the two domains [67] may be utilised to improve temperature uniformity.
- *Dynamic stability.* In the absence of thermostat and external loading, the interatomic potential-based internal energy in the atomistic domain is conserved, yet the same is not necessarily true for the continuum domain and the domain interface. On the one hand, an energy-based method may take the derivative of the energy as the 'force', which may not be the physically motivated force (e.g. the interatomic potential-based atomic force in atomistics) in the force-based dynamic formulation. On the other hand, the force-based methods, while having well-defined forces on all DOFs, have no well-defined total energy and may converge to unstable equilibrium states [13]. Junge et al. [68] found that the displacement-based atomistic/continuum coupling in a fully-dynamic setting, e.g. that in dynamic CADD [47], is unstable without damping, due to the difference between the linear interactions in the continuum domain and the nonlinear interactions in the atomistic domain. This

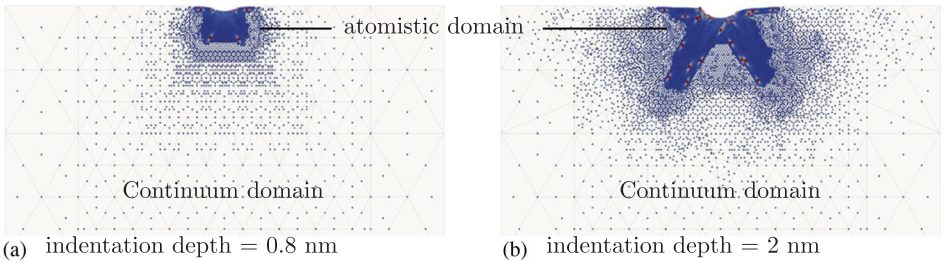

Figure 1. Snapshots of a QC simulation of nanoindentation on a Cu single crystal at a loading rate of 2×10^4 m/s. Atoms in the atomistic domain, as well as repatoms, sampling atoms, and element boundaries in the continuum domain, are in blue; dislocations identified by the centrosymmetry parameter [73] are in red. To address the dislocations that glide away from the indenter, some elements in (a) are refined to atomic-scale in (b). Reproduced with permission from [74].

suggests that in these methods, either a harmonic buffer layer or a thermostat is required to stabilise the atomistic/continuum domain interface at finite temperatures.

- *Spurious wave reflection.* While many efforts have been made to define temperature and maintain stability in the continuum domain, some researchers, e.g. Cai et al. [69], E and Huang [70], Yang et al. [71], and Ramisetti et al. [72] focused on improving the transmission of waves across the atomistic/continuum domain interface. It is known that wave propagation originated in the atomistic domain may not be fully transmitted to the continuum domain and may be reflected back, resulting in a localised, non-physical heating in the former [12], for several reasons: (i) different governing equations lead to differences in vibrational properties between the atomistic and continuum domains, resulting in aphysical scattering at the interface [48]; (ii) the continuum domain, with a lower numerical resolution that may be due to a larger characteristic length of the elements, does not naively receive all wave information from the atomistic domain that has a finer resolution and allows a shorter wavelength; and (iii) the pad region in the continuum domain, which is used to provide boundary conditions for the atomistics, usually lacks thermal motion which may have consequences on the dynamics of adjacent atoms.

Mesh refinement

The pre-partitioned simulation cell in domain decomposition methods works well when dislocations and heat follow prescribed paths or when the spatial distribution of areas of interest is invariant. In reality, however, the locations and paths of dislocations/heat are difficult to predict *a priori*. Since a domain decomposition multiscale simulation concerns domains of both discrete and continuum nature, a large numerical error may occur when the system evolves if the continuum domain, which may not explicitly admit dislocations and/or short-wavelength heat carriers, is not converted to atoms on time. Therefore, it is crucial for most atomistic/continuum coupling methods to re-partition the continuum domain down to the atomic-scale on-the-fly and adjust the domain interface accordingly; this is especially important in time-dependent dynamic problems [4]. We remark that besides the domain decomposition methods, the mesh refinement issue is also relevant to hierarchical methods, e.g. AtC [21], in which the continuum domain may employ a finer mesh as needed.

Depending on whether lattice defects (e.g. dislocations and point defects) are permitted in the continuum, mesh-refining atomistic/continuum coupling methods can be classified into two types. Among the five multiscale methods reviewed here, BDM and QC belong to the first type, in which the continuum domain needs to be refined locally to atomic-scale fidelity to address defects, as shown in Figure 1. As a consequence, the DOFs in a simulation scale with the defect volume, even with the assistance of mesh coarsening. In this spirit, coarse elements in the continuum domain, which do not naively support short-wavelength heat carriers, may need to be refined to finer elements or atoms in the presence of heat conduction, depending on the specific wavelength. The second type includes AtC, CAC, and CADD, whose continuum domains describe heat or defects by either constitutive relations, discontinuous elements, or lattice elasticity with defect field interactions. Accordingly, mesh refinement in the second type of method is less demanding than that in the first type. Still, mesh refinement is needed in some cases, because (i) point defects are not explicitly accounted for in the continuum domain in CAC and CADD and (ii) only dislocations on slip planes that are between discontinuous elements are exhibited in CAC. For both types of mesh-refining methods, one common challenge is the geometric complexity of the mesh and its adaption, due to either the interelement compatibility requirement and/or enrichment strategies in the continuum, or the information passing techniques between the two domains [75]. In addition, in cases where continuous finite elements with high-order shape functions are used to represent a defected lattice, the assignment of atom coordinates from a continuum may not be unique and straightforward [12].

Table 1. Summary and comparisons of the five atomistic/continuum coupling methods reviewed in this paper. In the two rows associated with 'heat conduction', P and E stand for phonon- and electron-mediated heat conduction, respectively. Key references are provided.

	AtC	BDM	CAC	CADD	QC
Handshake region	Yes[a]	Yes	No	No	No
Coupling boundary condition	Strong	Weak	Strong	Strong	Strong
Statics	No	Yes [22]	Yes [34]	Yes [24]	Yes [25]
Zero *T* dynamics	No	Yes [46]	Yes [76]	Yes	Yes
Finite *T* equilibrium dynamics	Yes	Yes [46,77]	Yes [78]	Yes [47,79,80]	Yes [61,63,81,82]
Finite *T* non-equilibrium dynamics	Yes [21,83]	Yes [46,84]	Yes [85]	No	Yes [62,82,86]
Dislocations in the continuum	No	No[b]	Yes [23,34]	Yes [24,87]	No
Dislocations across the interface	No	No	Yes [23,34]	Yes [24,87]	No
Heat conduction in the continuum	P [21] & E [88]	P [46,84]	P [89–91]	No	P [82,86]
Heat conduction across the interface	P [21] & E [88]	P [46,84]	P [85,92,93]	No	P [82,86]
Dislocation/phonon interactions	No	No	Yes [89,94]	No	No

[a]In AtC, the atomistic domain is overlaid on part of [21] or the whole continuum domain [83]. [b]In extended finite element method (XFEM)-BDM [95,96], a large portion of the slipped region, but not the dislocation itself, is solved by XFEM.

Key characteristics of the five atomistic/continuum coupling approaches

As we focus on their applications to dislocations, heat conduction, and dislocation/phonon interactions in a problem-centric manner in this paper, we present a brief discussion of key characteristics of the five atomistic/continuum coupling approaches in this section. Below, we define the handshake region as the transitional region within which atoms and finite elements coexist, while the pad region as the one that is only in the atomistic or continuum domain and provides boundary conditions for the other. If the pad region is constrained to move as if it were glued to the domain in which it resides, the atomistic/continuum coupling boundary condition is 'strong compatibility'; otherwise, it is 'weak compatibility' [13]. A summary of the five methods is presented in Table 1; the readers are referred to the original articles for details of the mathematical formulation, numerical implementation, and full capabilities of these methods.

Atomistic-to-Continuum

The AtC method was proposed to effect the two-way temperature coupling between the MD and continuum domains in heat conduction [21]. In AtC, the MD domain is established to capture nanoscale structures for which a continuum description is inappropriate. The MD domain is then overlaid and surrounded by a continuum domain with finite element representation, as shown in Figure 2, similar to an earlier method proposed by Schall et al. [97].

On the one hand, the continuum domain serves as a heat bath by providing a pad region with ghost atoms in the continuum as boundary conditions for the atomistic domain, i.e. [21],

$$m_k \ddot{\mathbf{R}}_k = \mathbf{F}_k - \frac{1}{2} m_k \dot{\mathbf{R}}_k \sum_{\xi}^{N_{\text{npe}}} \Phi_{k\xi} \lambda_\xi(t), \qquad (4)$$

where $\ddot{\mathbf{R}}_k$ is the acceleration vector of the kth atom, $\mathbf{F}_k$ is the interatomic potential-based atomic force on the kth atom, $\Phi_{k\xi}$ is the shape function of node ξ at the kth atom, t is the time, and $\lambda_\xi(t)$ is the time-dependent, continuum domain-informed nodal coefficient chosen to enforce conservation of total energy.

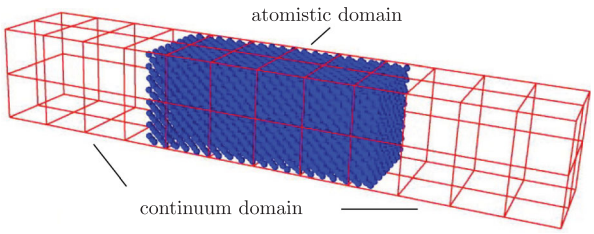

Figure 2. An AtC simulation cell with atoms and finite elements represented by blue spheres and red grid, respectively. Reproduced with permission from [21].

On the other hand, a temperature field in the continuum domain, T_ν, is coupled with that in the atomistic domain, T_k, by minimising their squared difference; as a result, for all nodes ξ [21],

$$\sum_{\nu}^{N_{\text{npe}}} \left(\sum_{k}^{N_{\text{ape}}} \Phi_{k\xi} \Phi_{k\nu} \Delta V_k \right) T_\nu = \sum_{k}^{N_{\text{ape}}} \Phi_{k\xi} \Delta V_k T_k, \qquad (5)$$

where ν is a node and ΔV_k is the volume of the kth atom. By assuming Fourier's law in the continuum with parameters (e.g. thermal conductivity and heat capacity) that may be informed by time-filtered atomistics, thermal information flows in both directions. Note that with some complex interatomic potentials, the spurious force at the domain interface needs to be corrected [13]. The AtC method has been implemented into the atomistic simulation software LAMMPS[1] [33].

Bridging Domain Method

BDM employs a handshake region with Lagrange multipliers to enforce a weak compatibility between the atomistic and continuum domains, as illustrated in Figure 3; indeed, it is the only method among the five reviewed in this paper that imposes a weak

[1]http://lammps.sandia.gov/doc/fix_atc.html

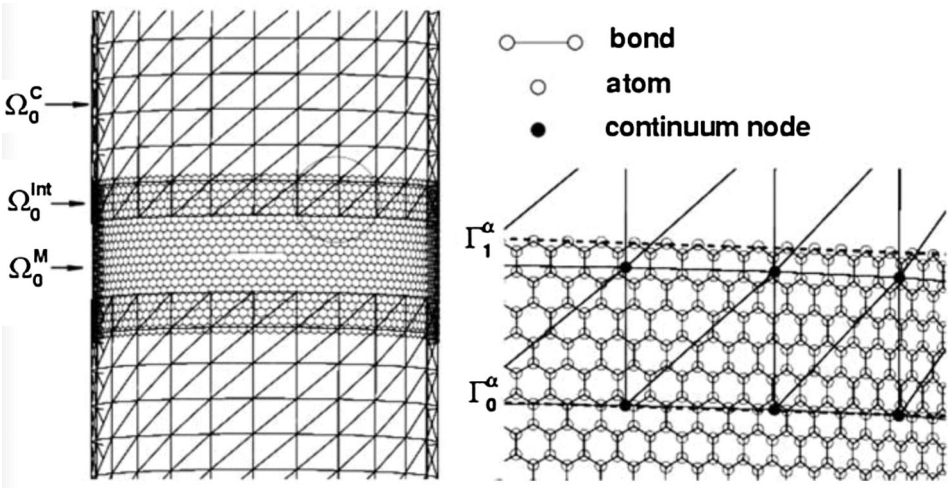

Figure 3. A BDM simulation cell for nanotube. The atomistic and continuum domains are labelled by Ω_0^M and Ω_0^C, respectively; the handshake region Ω_0^{Int} is bounded between two edges Γ_0^α and Γ_1^α. Reproduced with permission from [46].

compatibility across the domain interface (Table 1). The original BDM adopted an energy-based formulation to connect an MS model with a continuum [22]; later, it was extended to dynamics [46], finite temperature [98], and force-based formulations [99,100]. In both static and dynamic settings, in the handshake region, a scaling parameter α is introduced, and the total Hamiltonian H, constructed with the help of the augmented Lagrangian method to impose the displacement compatibility between atoms and nodes within a penalty β, is [22,46]

$$H = (1-\alpha)H^{\mathrm{AD}} + \alpha H^{\mathrm{CD}} + \sum_{k}^{N_{\mathrm{atom}}} \boldsymbol{\lambda}_k^{\top}\mathbf{g}_k + \frac{1}{2}\sum_{k}^{N_{\mathrm{atom}}} \beta \mathbf{g}_k^{\top}\mathbf{g}_k, \tag{6}$$

where H^{AD} and H^{CD} are Hamiltonians of the atomistic and continuum domains, respectively, $\mathbf{g}_k$ is the difference in the displacement vector between the atom and the continuum material point at the kth atomic site, and $\boldsymbol{\lambda}_k$ is a vector of Lagrange multipliers whose component is related to the displacement of the kth atom. In this way, the handshake region filters the wave components with short wavelength and has been demonstrated to effectively suppress spurious wave reflection [46] with conserved linear and angular momenta [101]. Compared with the other four methods reviewed in this paper, BDM focuses more on the coupling scheme itself which has been borrowed to integrate a continuum domain with discrete elements [102].

In the absence of heat conduction, the balance of linear momentum is ensured in the continuum domain with the constitutive relation constructed via the Cauchy-Born rule; for heat conduction problems, assuming that all deformations are reversible, an additional energy equation is introduced, i.e. [46],

$$\rho\bar{c}\dot{T} = \kappa\nabla^2 T + S, \tag{7}$$

where ρ is the mass density, $\bar{c}$ is the specific heat, κ is the thermal conductivity, and S is the internal heat source. Note that $\bar{c}$ and κ are empirical parameters informed by experiments and/or other calculations.

In the standard BDM, part of the continuum domain has to be refined to atomic-scale to encompass evolving lattice defects such as dislocations [103]. However, the increasing DOFs as a result of this refinement may be lowered by employing an XFEM-based continuum domain [104] to accommodate a large portion of the slipped region but not the dislocation [95,96]. This new method, termed XFEM-BDM, has been extended to studying dynamic crack propagation in which the crack tip is within an atomistic domain while a large portion of the fractured surface is numerically solved by XFEM [105,106].

Concurrent Atomistic–Continuum

The CAC method employs a unified atomistic–continuum formulation that is built upon the atomistic field theory, with governing equations being [107,108]

$$\frac{\mathrm{d}\rho^\alpha}{\mathrm{d}t} + \rho^\alpha(\nabla_{\mathbf{x}}\cdot\mathbf{v} + \nabla_{\mathbf{y}^\alpha}\cdot\Delta\mathbf{v}^\alpha) = 0, \tag{8}$$

$$\rho^\alpha\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{v}+\Delta\mathbf{v}^\alpha) = \nabla_{\mathbf{x}}\cdot\mathbf{t}^\alpha + \nabla_{\mathbf{y}^\alpha}\cdot\boldsymbol{\tau}^\alpha + \mathbf{f}_{\mathrm{ext}}^\alpha, \tag{9}$$

$$\rho^\alpha\frac{\mathrm{d}e^\alpha}{\mathrm{d}t} = \nabla_{\mathbf{x}}\cdot\mathbf{q}^\alpha + \nabla_{\mathbf{y}^\alpha}\cdot\mathbf{j}^\alpha + \mathbf{t}^\alpha : \nabla_{\mathbf{x}}(\mathbf{v}+\Delta\mathbf{v}^\alpha) + \boldsymbol{\tau}^\alpha : \nabla_{\mathbf{y}^\alpha}(\mathbf{v}+\Delta\mathbf{v}^\alpha), \tag{10}$$

where $\mathbf{x}$ is the physical space coordinate of the continuously distributed lattice, $\mathbf{y}^\alpha$ ($\alpha = 1,2,\ldots,N_a$ with N_a being the total number of atoms in a unit cell) is the subscale internal variable corresponding to the position

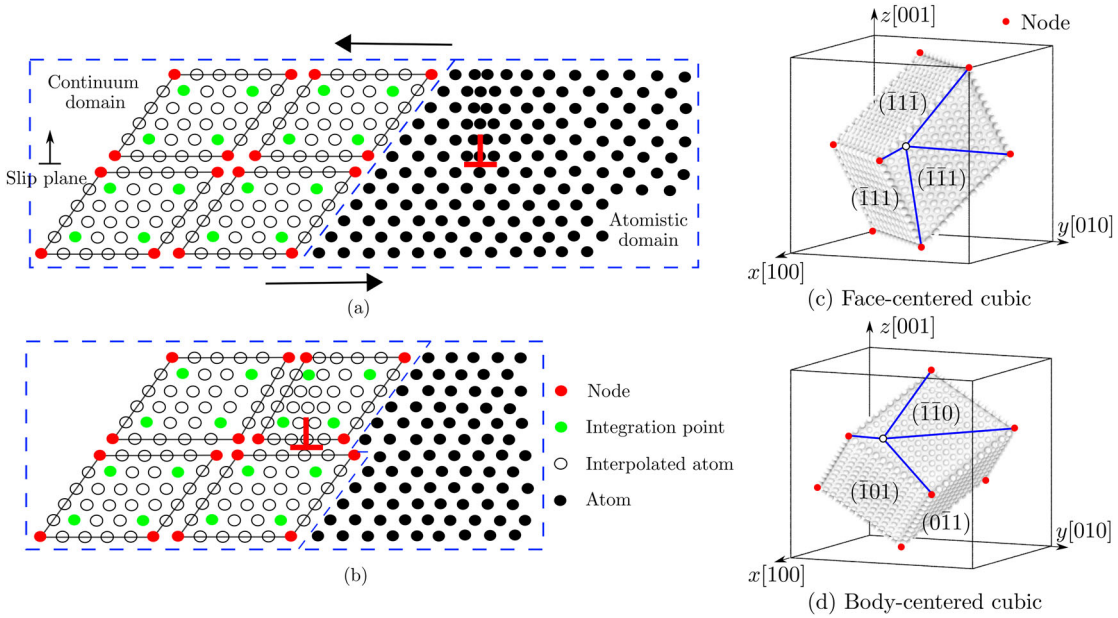

Figure 4. (a–b) A 2D CAC simulation domain consisting of a continuum domain (left) and an atomistic domain (right). In (a), the atomistic domain contains an edge dislocation (red ⊥) which, upon applying a shear stress to the simulation cell, migrates into the continuum domain in (b), where the Burgers vector spreads out between discontinuous finite elements. (c–d) In 3D, elements have faces on {111} planes and on {110} planes in a face-centred cubic (FCC) and a body-centred cubic (BCC) lattice, respectively. The positions of atoms (black open circles) within each element are interpolated from the nodal positions (red filled circles). Reproduced with permissions from [34,35].

of atom α relative to the mass centre of the lattice located at $\mathbf{x}$, ρ^α, $\rho^\alpha(\mathbf{v}+\Delta\mathbf{v}^\alpha)$, and $\rho^\alpha e^\alpha$ are, respectively, the local density of mass, linear momentum, and total energy, $\mathbf{v}$ is the velocity field, $\mathbf{v}+\Delta\mathbf{v}^\alpha$ is the atomic-level velocity, $\mathbf{f}^\alpha_{\text{ext}}$ is the external force field, $\mathbf{t}^\alpha$ and $\mathbf{q}^\alpha$ are, respectively, the momentum and heat flux tensors due to the homogeneous distortion of lattice cells, $\boldsymbol{\tau}^\alpha$ and $\mathbf{j}^\alpha$ are, respectively, the momentum and heat flux tensors resulted from the reorganisation of atoms within the lattice cells and represent the components of stress and heat flux due to the inhomogeneity at the sub-lattice scale.

In the continuum domain in CAC, non-local elements can have discontinuities between them, with the underlying interatomic potential as the only constitutive relation [109]; the faces of elements are assumed to lie on the slip planes or cleavage planes of the lattice, as shown in Figure 4. In this way, with no 'ghost forces' at the atomistic/continuum domain interface in undeformed and affinely deformed configurations, CAC admits certain lattice defects such as dislocations, intrinsic stacking faults, and cracks, but not extrinsic stacking faults and twins [110], in the continuum domain. As such, CAC enables defect movement and heat conduction between the two domains without essential remeshing operations [111]. Both static [34] and dynamic formulations [23] of CAC have been proposed and implemented, e.g. into PyCAC[2] [35]. The CAC method has been utilised to simulate static dislocation properties [34,111], conservative dislocation movement [4,23,59,76,91,109,110,112–119], heat conduction [85,92,93,120], and dislocation/phonon interactions [89,91,94,121] in a wide range of metallic, semiconductor, and polyatomic ionic materials.

Coupled Atomistic/Discrete-Dislocation

The CADD method [24] was proposed to allow dislocation movement between the atomistic and continuum domains. The original CADD method was limited to 2D quasistatics at 0 K [122]; later, dynamic CADD at finite temperatures was introduced [47]. Pad atoms on the continuum side provide boundary conditions for MS/MD calculations in the atomistic domain, as shown in Figure 5. The continuum domain is subject to reduced order continuum models for elastic stress fields of dislocations interactions at long range (i.e. linear elasticity), as in discrete dislocation dynamics (DDD), which drives the motion of the ith dislocation using the Peach-Koehler (PK) force $\mathbf{F}_i$, i.e. [124],

$$\dot{\mathbf{R}}_i = M_i(\mathbf{F}_i), \tag{11}$$

$$\mathbf{F}_i = (\boldsymbol{\sigma}\cdot\mathbf{b}_i)\times\mathbf{l}_i, \tag{12}$$

$$\boldsymbol{\sigma}_{\text{dis}} = \sum_{j=1,j\neq i}^{N_{\text{dis}}} \boldsymbol{\sigma}_j(\mathbf{b}_j,\mathbf{l}_j,\alpha_{\text{ela}}), \tag{13}$$

where $\dot{\mathbf{R}}_i$ is the velocity of the ith dislocation, $\mathbf{b}_i$ is the Burgers vector of the ith dislocation, $\mathbf{l}_i$ is the unit vector

[2]http://www.pycac.org/

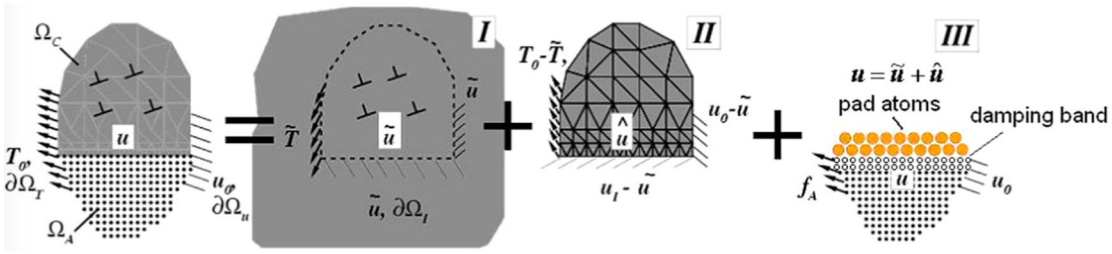

Figure 5. A 2D schematic illustration of the solution procedure for CADD. The total problem is divided into a continuum domain (Ω_C) and an atomistic domain (Ω_A) coupled together by 'strong compatibility'. The continuum domain is split into two subproblems: the first (I) treats all continuum dislocations as line defects in an infinite medium, resulting in the displacement field $\tilde{\mathbf{u}}$ and boundary traction $\tilde{\mathbf{T}}$, while the second (II) consists of a dislocation-free linear elastic finite element problem subject to the true displacement field $\mathbf{u}_0$ and boundary traction $\mathbf{T}_0$ minus those of the first subproblem. In III, the pad atoms residing in the continuum, along with $\mathbf{u}_0$ and $\mathbf{T}_0$, provide boundary conditions for the atomistic domain; a Nosé–Hoover thermostat is applied to the atoms in the damping band to reduce the spurious wave reflection at the atomistic/continuum domain interface, while other atoms are left unthermostated. Reproduced with permission from [123].

along the ith dislocation line direction, N_{dis} is the total number of dislocations in the system, and $\boldsymbol{\sigma}$ results from linear superposition of all stress tensors applied on the ith dislocation, among which the most important one is usually the stress fields caused by all other dislocations in the system, $\boldsymbol{\sigma}_{\text{dis}}$. The stress field of the jth dislocation, $\boldsymbol{\sigma}_j$, as a function of $\mathbf{b}_j$, $\mathbf{l}_j$, and some elastic constants α_{ela}, can be calculated using linear elasticity theory [124]. Certain parameters, including the dislocation character angle-specific mobility law M (which may be non-linear with respect to $\mathbf{F}$ [125]), core radius (which is needed in calculating the dislocation stress fields [126]), core energy (which is added to the elastic energy [111]), and short-range interactions, are usually informed by atomistic simulations [127].

In dynamic setting at finite temperatures, the atomistic domain employs a Nosé–Hoover thermostat [64–66]; the continuum domain is associated with pre-defined temperature-dependent properties yet accepting no heat dissipated by the atomistic domain [47]. However, a standard thermostat may improperly damp out any non-equilibrium behaviour, especially so in small atomistic systems, which are usually the case in atomistic/continuum coupling simulations. To better replicate the non-equilibrium character in atomistics, later versions of dynamic CADD leave the majority of the atomistic domain unthermostated, i.e. the atoms are assigned initial velocities and then evolve according to the microcanonical ensemble; for atoms in a narrow damping band near the atomistic/continuum domain interface (Figure 5), either a Langevin-like dynamics [79] or a Nosé–Hoover thermostat [80] is applied. The purpose of this damping band, within which atoms are gradually damped from interior to the domain interface where all atoms have a zero velocity, is to reduce the spurious wave reflection at the interface [79]. Recently, CADD was extended to 3D in which curved dislocation segments can be transferred across the atomistic/continuum domain interface [128–130]. Note that CADD was not designed for heat conduction, but specifically for conservative dislocation movement [47,80,123,131–135].

Quasicontinuum

QC, one of the most widely cited atomistic/continuum coupling methods that inspired many other multiscale modelling approaches [136,137], accomplishes atomistic coarse-graining by using a reduced set of representative atoms (repatoms) μ to link slave atoms k which follow repatoms via a Cauchy-Born rule, i.e. [25],

$$\mathbf{R}_k = \sum_{\mu}^{N_{\text{rep}}} \mathbf{\Phi}_{k\mu} \mathbf{R}_\mu, \tag{14}$$

where N_{rep} is the total number of repatoms in the system. The interatomic potential-based total energy E and force $\mathbf{F}$ on repatom μ are

$$E = \sum_{k}^{N_{\text{atom}}} E_k(\mathbf{R}_k) = \sum_{k}^{N_{\text{atom}}} E_k\left(\sum_{\mu}^{N_{\text{rep}}} \mathbf{\Phi}_{k\mu} \mathbf{R}_\mu\right), \tag{15}$$

$$\mathbf{F}_\mu = -\frac{\partial E}{\partial \mathbf{R}_\mu} = -\sum_{k}^{N_{\text{atom}}} \frac{\partial E}{\partial \mathbf{R}_k} \frac{\partial \mathbf{R}_k}{\partial \mathbf{R}_\mu} = \sum_{k}^{N_{\text{atom}}} \mathbf{F}_k \mathbf{\Phi}_{k\mu}, \tag{16}$$

which require computing the energy and forces of all slave atoms, despite the reduced DOFs from N_{atom} to N_{rep}. Therefore, summation rules, including node-based cluster summation in force-based [138] and energy-based QC [139], as well as quadrature-type summation [37,140], have been introduced to replace the sum over index k in Equations (15) and (16) by a weighted sum over selected sampling atoms (Figure 6), hence reducing the cost of ensemble sampling for force or energy. In *local* QC, a correction needs to be applied to eliminate the 'ghost force' at the atomistic/continuum domain interface [36], which is minimised in cluster QC [138] or fully *non-local* QC [37].

Over the last two decades, numerous dynamic formulations of the QC method, collectively termed 'hot-

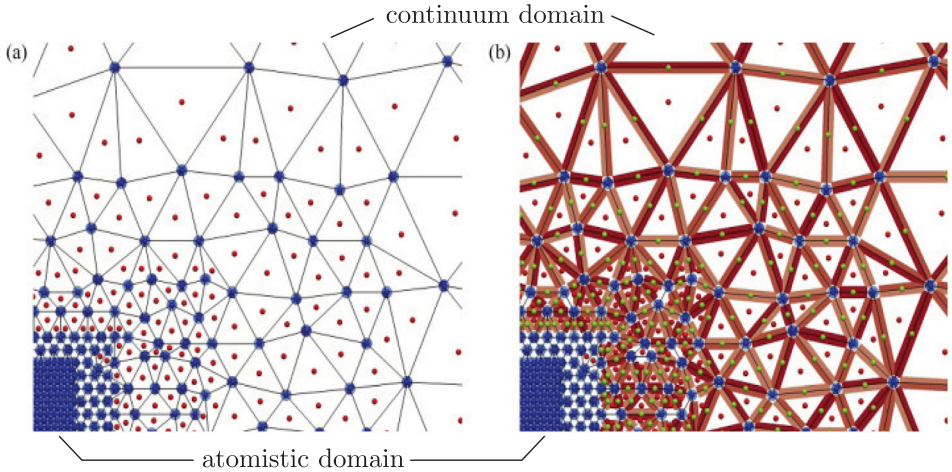

Figure 6. A 2D illustration of a QC simulation cell with different summation rules. In both (a) and (b), atoms in the atomistic domain and repatoms and element boundaries in the continuum domain are in blue; inner-element sampling atoms are in red with the white regions representing their weights within each element. In (b), sampling atoms (green) also exist at edge midpoints, with red regions representing their weights along the same edge. Reproduced with permission from [37].

QC' [60–63,81,82,86] have been proposed. More recently, 'hyper-QC' [57] was developed by introducing hyperdynamics [51] into 'hot-QC' to coarse-grain both length and timescales for equilibrium and quasi-equilibrium problems. However, in all these QC flavours, like standard BDM, lattice defects such as dislocations cannot pass through the continuum domain, but requiring adaptive refinement to full atomic resolution or *a priori* assignment of the atomistic domain where dislocation migration and interactions are expected to occur [74,141]. For this reason, we only review the application of QC to heat conduction [142–145] in this paper. Additional information of the QC method can be found on a dedicated website[3].

Dislocations

The motions of dislocations, linear crystalline defects with cores that are nanometre wide, control the plastic deformation of crystalline materials. A dislocation has two properties, a line direction $\mathbf{l}$ and the Burgers vector $\mathbf{b}$, the latter of which describes the magnitude and direction of distortion to the lattice. The angle between $\mathbf{l}$ and $\mathbf{b}$ is the character angle of a dislocation; accordingly, two ends of the spectrum are an edge dislocation with $\mathbf{b} \perp \mathbf{l}$ and a screw dislocation with $\mathbf{b} \parallel \mathbf{l}$, as shown in Figure 7. Mixed-type dislocations, which possess character angles between 0° and 90°, are prevalent in plastically deformed crystals, yet their key characteristics, such as the core structure and core energy, cannot simply be extrapolated from those of edge and screw dislocations [125,147]. Thus, in a given material, a dislocation with a given $\mathbf{b}$ on a given slip plane S_0 can theoretically posses infinite numbers of character angles by infinitesimally varying $\mathbf{l}$, necessitating infinite numbers of direct modelling.

In most atomistic/continuum coupling approaches, lattice defects such as dislocations are not permitted in the continuum domain whose behaviour is usually limited to hyperelasticity. As dislocations approach the domain interface from the atomistic side, either part of the continuum domain adjacent to the slip plane is refined to atomic-scale (e.g. in AtC, standard BDM, and QC) or only the elastic component of the atomistic displacement is passed to the continuum domain as elastic displacement boundary conditions (e.g. in the modified ESCM [135]), effectively annihilating the dislocations at the domain interface. In this section, we focus on methods that admit dislocations in both atomistic and continuum domains, as well as a two-way exchange of dislocations between the two domains. Examples of such methods are CAC and CADD, which have more predictive character than one-way linking strategies. We will also discuss XFEM-BDM, which may be extended to realise such two-way exchange. In all three methods, a coarse-grained description of dislocations is made possible by enriching the physics in the continuum.

Movement of dislocations can be classified into conservative and non-conservative types, referring to dislocation movement that takes place within and out of the slip planes, respectively [124]. Note that the conservative movement of a dislocation is not constrained to the same slip plane. For example, the cross-slip process by which a screw dislocation moves from one slip plane to another is conservative and has been successfully simulated in the continuum domains in CAC [109] and CADD [148]. While theoretically feasible, cross-slip of a screw dislocation at the atomistic/continuum domain interface and dislocation gliding along the interface have not been tested in simulations using

[3]http://qcmethod.org/

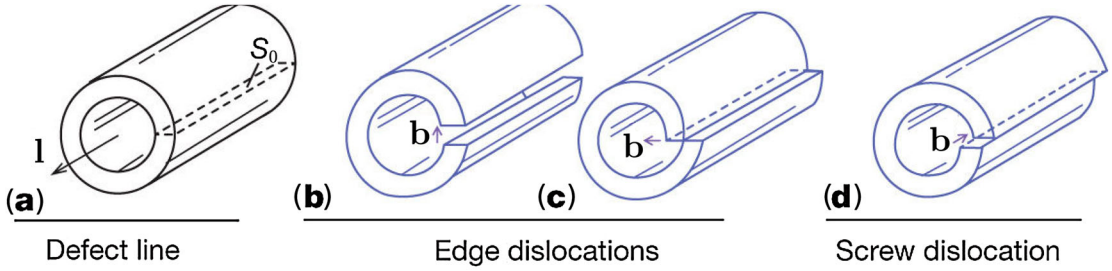

Figure 7. Illustrations of Volterra dislocations. (a) A reference cylinder with defect line **l** and cut surface S_0. (b–c) Edge dislocations with Burgers vector **b** ⊥ **l**. (d) A screw dislocation with Burgers vector **b** ∥ **l**. Reproduced with permission from [146].

any of these methods, to the best of our knowledge; in practice, cross-slip mostly occurs in individual domains. Additionally, most atomistic/continuum coupling approaches cannot simulate non-conservative movement of dislocations (i.e. climb) across the domain interface, except the recently proposed discrete diffusion-molecular dynamics (DDf-MD) method [149]. In DDf-MD, the continuum domain employs continuum diffusion equations to control the site-by-site diffusion of point defects that help dislocation climb in the atomistic domain [150], instead of providing an explicit description of dislocation ensembles as in CAC and CADD. In other words, it is the point defects, not dislocations, that are passed across the domain interface in DDf-MD, while only the atomistic domain is able to explicitly account for dislocation lines. We note that non-conservative movement of dislocations can be described in a continuum [151,152], yet we are not aware of any attempt in the literature to couple it with atomistics. Therefore, in the following, we focus on the description of dislocations in the continuum in the next subsection and the conservative dislocation movement on the same slip plane across the atomistic/continuum domain interface in the subsection after next.

Dislocations in the continuum domain

In the atomistic domain, dislocations can be created by applying the corresponding isotropic or anisotropic elastic displacement fields to the atoms [153]. The same procedure is employed in the continuum domain in CAC, except that, instead of atoms, the nodes of finite elements are displaced. If the energy minimised dislocation core structure is desired, an MS or a quasistatic CAC simulation [34] can be carried out subsequently. Another method that also introduces the dislocation displacement field into the continuum is XFEM, in which the displacement field is instantiated through a step function across the active slip planes [154]; an additional core enrichment may be added in the neighbourhood of the dislocation to better represent the local core structure [155,156]. On the contrary, dislocation dynamics in the continuum domain in CADD is dictated by DDD, which makes use of the long-range stress fields of dislocations, instead of explicitly accounting for the displacement fields.

Within the classical local continuum theory framework, it is difficult to attain an accurate dislocation core description. The challenges originate in essence from the continuum assumption which is inconsistent with the discrete and atomistic nature of dislocations [157]. Moreover, analytic solutions, of either the displacement field (e.g. in XFEM) or the stress field (e.g. in DDD), do not exist for fully anisotropic elastic media [158]. Consequently, the continuum is deemed inadequate in representing dislocations, especially when an accurate core description is desired. For example, it seems straightforward to propose an atomistic/continuum coupling method that passes dislocations between an atomistic domain and an XFEM-based continuum domain, which would be similar to CAC and CADD. However, such a method has not been developed, to the best of our knowledge. Instead, in XFEM-BDM [95,96], the regions around the dislocations are always rendered in atomistic resolution, while a large portion of the slipped region, whose lattice deformation is simpler than that of the dislocation, is accommodated via a step function in XFEM. In effect, some atoms adjacent to the slip plane in standard BDM are coarsened to enriched finite elements in the XFEM-BDM model, which contains fewer DOFs than the former, as shown in Figure 8. We remark that XFEM-BDM has not been extended to 3D.

In CAC, to facilitate dislocation nucleation and migration in the continuum domain, discontinuous finite elements are employed with all faces lying on the slip planes, e.g. {111} planes in FCC and {110} planes in BCC lattices, respectively, as shown in Figure 4(c,d). Between elements, neither displacement continuity nor strain compatibility is required. Within each element, lattice defects are not allowed and the displacement field has C^1 continuity. To numerically calculate the balance equations, Galerkin method and Gaussian quadrature are employed, with each element containing a fixed number of integration points – 125 in a second nearest neighbour type of element [34]–

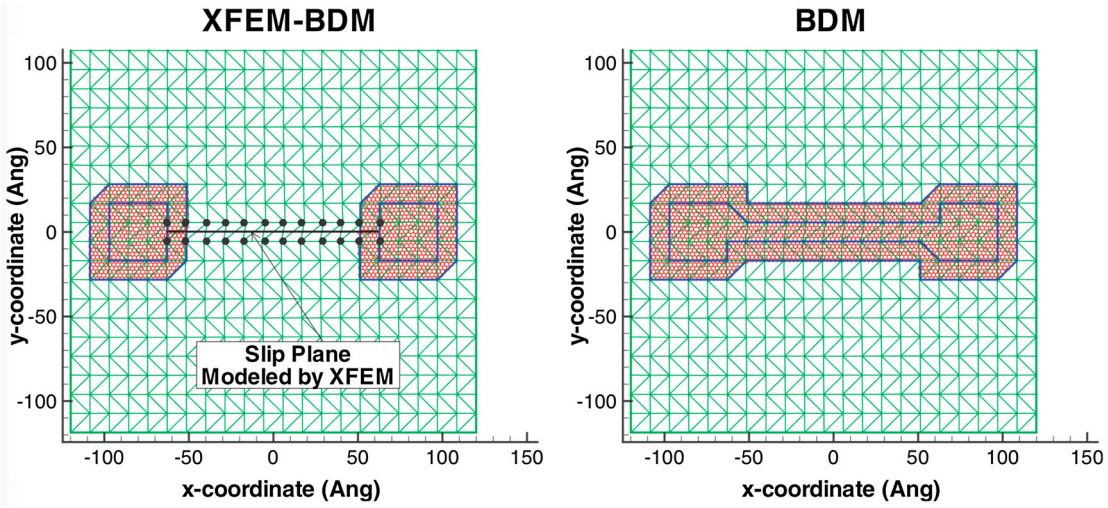

Figure 8. A graphene sheet containing a pair of edge dislocations: (left) XFEM-BDM and (right) standard BDM. Green and blue lines denote the finite elements and the Lagrange multiplier meshes, respectively. Black circles are the nodes enriched by the step function. Reproduced with permission from [95].

regardless of the element size instantiated by N_{ape}. Consequently, when $N_{\text{ape}} = 125$, all atoms are integration points, introducing only the discretisation error; when $N_{\text{ape}} = 729$, both discretisation and integration errors take effect, resulting in a larger difference from atomistics, as shown in Figure 9. Prior convergence analyses found that CAC predictions properly converge to the fully atomistic results as the finite element size is reduced [23,34,112,121]. We remark that dislocation arrays in the continuum domain in CAC, regardless of N_{ape}, have the same Burgers vector **b**, line direction **l**, total number of

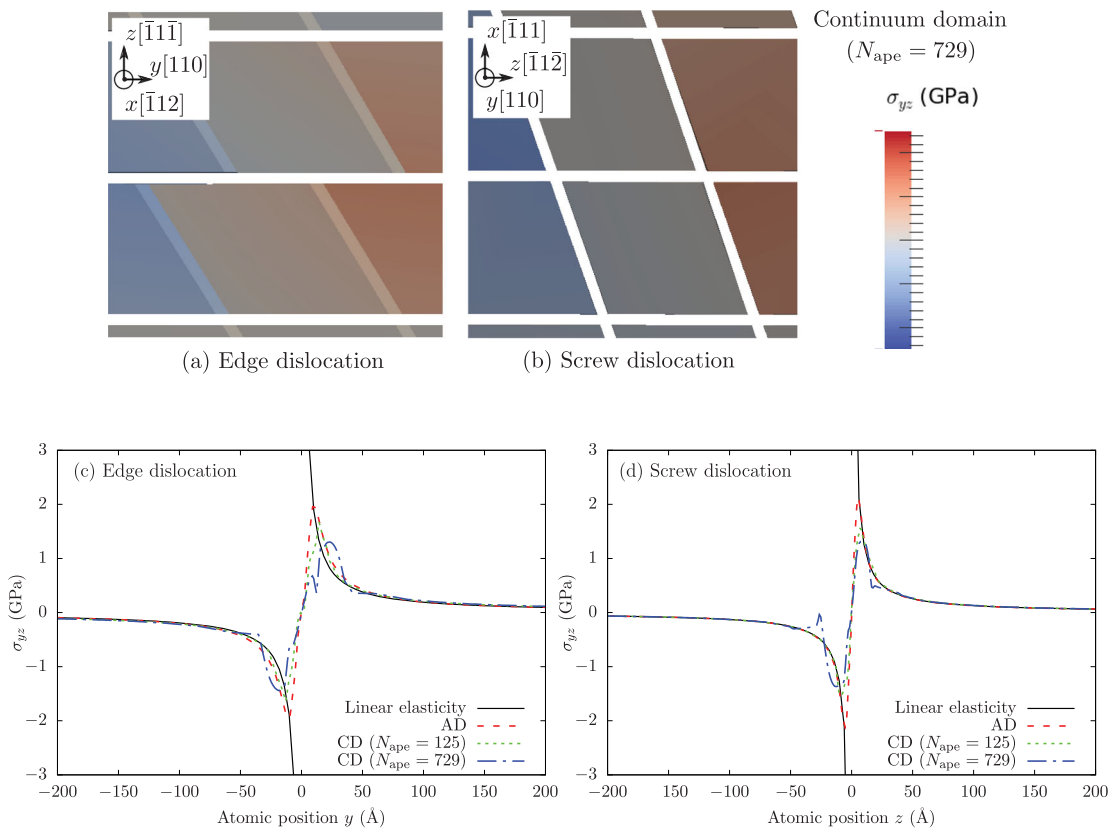

Figure 9. Snapshots of the shear stress (σ_{yz}) fields around a single dislocation with (a) pure edge and (b) pure screw character in the continuum domain in CAC for Al, with the Mishin embedded-atom method potential [159]. Periodic boundary conditions are applied along the dislocation line direction, i.e. the x axis in (a) and the y axis in (b). (c–d) σ_{yz} profiles of a single dislocation along the y (edge) and z (screw) direction predicted by the atomistic domain (AD), the continuum domains (CD) with different element sizes N_{ape}, and the isotropic linear elasticity.

dislocations N_{dis}, and elastic constants α_{ela} as those in the atomistic domain, suggesting that the PK force is correctly reproduced, according to Equations (12) and (13). However, compared with atomistics, the continuum domain in CAC generally predicts a wider stacking fault width, a lower stacking fault energy, a flatter dislocation core, a larger core radius, a higher core energy, and a lower Peierls stress [75]. For example, when $N_{ape} \approx 10{,}000$, the stacking fault width of a 60° dislocation predicted by the continuum domain is about twice that in atomistics [34]. The systematic coarse-graining error, together with the fact that dislocations can only be accommodated between finite-sized elements but not within, suggest that CAC may not be suitable for problems requiring an accurate description of dislocation cores in the presence of high dislocation density.

Compared with the static dislocation properties, the dynamics of dislocations is more pertinent to engineering applications. As will be discussed in the section after next, a moving dislocation scatters thermal phonons that are already in the lattice while also radiating lattice waves. In addition, at high strain rates ($\geq 10^6$ s^{-1}), the inertia effects on the motion of dislocations, which are ignored in classical DDD, become important [160]; the stress fields of a supersonic dislocation is no longer symmetric with respect to the dislocation centre [91,161], as shown in Figure 10. All these complex dynamic features of fast moving dislocations, especially the velocity/temperature-dependent core properties and energy radiation [162], may be integrated into DDD and XFEM to enable full non-equilibrium elastodynamics of dislocations in the continuum. Note that in its current form, finite temperature CADD [47,79,80] employs a quasistatic finite element solution, and so the continuum is always in equilibrium. By comparison, despite with a higher dislocation mobility accompanied with an increasing element size [91], CAC naturally replicates the inertia effect and other elastodynamic properties of moving dislocations by introducing the interatomic potential into the continuum domain as the only constitutive rule [90,91].

Dislocation movement across the atomistic/continuum domain interface

One major advantage of CAC and CADD is the allowance of the two-way dislocation movement between the atomistic and continuum domains. In CAC, the dislocation migration is achieved by rearranging nodes and atoms across the domain interface (Figure 4), a process enabled by having the same interatomic potential in both domains. Both quasistatic [34] and dynamic [113] dislocation migration across the domain interface have been realised in Cu and Al. When an extended dislocation, with a finite stacking fault width, sits right across the domain interface, the two partial dislocations will be in different domains and thus have asymmetric disregistry, as shown in Figure 11. It is shown that the domain interface only slightly alters the disregistry in its vicinity, and the dislocation has a correct core structure once it migrates into the atomistic domain. However, because displacement discontinuities in the continuum domain are only admitted between finite-sized elements, the number of possible slip planes there is effectively reduced with respect to the atomistic domain. As a result, when the dislocation pathway is not aligned with the interelement boundaries, the finite elements that potentially block the dislocation migration should either be split into two smaller ones with their boundaries along the dislocation path [163] or be refined to atomic scale [4]; otherwise, a dislocation may be reflected by the atomistic/continuum domain interface, glide along the interface before moving into interelement boundaries, or be pinned by the interface while new dislocations are nucleated between interelement boundaries [113]. In all, CAC is useful for exploring problems in which complex atomistic phenomena involving short-range dislocation reactions with lattice defects are limited to certain spatial regions, while only capturing long-range elastic interactions is required elsewhere. Examples of such CAC applications include interactions between dislocations and void [90], stacking fault [110], and grain boundary [76,118].

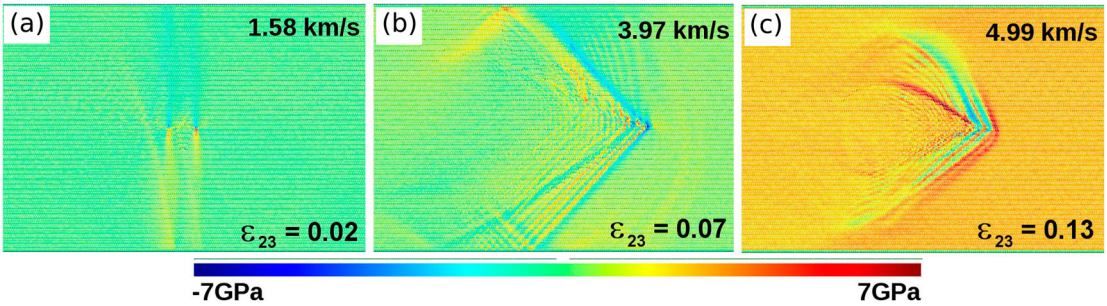

Figure 10. MD simulations of a fast moving edge dislocation in the (a) subsonic, (b) transonic, and (c) supersonic regimes in a Cu single crystal subject to a homogeneous in-plane shear. Atoms are coloured by the in-plane shear stress to highlight the Mach cones in (b) and (c). Reproduced with permission from [161].

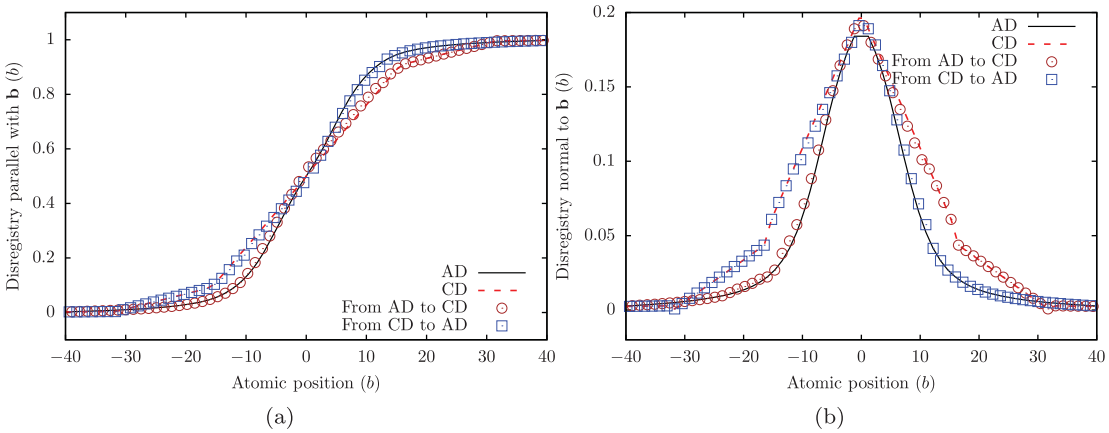

Figure 11. Disregistry profile of a static 60° dislocation in Cu, which sits right across the interface (with zero atomic position coordinate) between the atomistic (AD) and continuum domains (CD) with $N_{ape} = 2197$. The disregistry field is (a) parallel with and (b) normal to the Burgers vector. Results of a static dislocation in AD and CD, respectively, are given as references. Reproduced with permission from [34].

In CADD, different approaches for transferring dislocations across the atomistic/continuum domain interface are adopted in 2D and 3D systems, termed CADD2d and CADD3d, respectively [87]. In CADD2d, as shown in Figure 12, a detection band is introduced to identify a dislocation in the atomistic domain through recursively comparing its core structure with 'core templates' that are calculated offline in MS simulations. It follows that the original dislocation is annihilated and the same dislocation is re-built on the continuum side across the domain interface [122]; a similar strategy is used to realise the passing of a dislocation from the continuum domain into the atomistic domain. In both processes, the dislocation jump distance, with the help of a 'template method' that reduces the spurious force arising from the interactions of dislocations with the artificial domain interface, is usually on the order of a few nm [164]. Thus, only a near seamless two-way dislocation exchange is realised in CADD2d. Note that the AtoDis method [165] which, otherwise similar to CADD2d, uses the resolved shear stress at the atomistic/continuum domain interface to detect and transfer dislocations.

In CADD3d, besides the 'core templates', the mobilities of pure/mixed-type dislocations are calculated in advance in offline MD simulations. These MD-informed dislocation mobilities (Equation (11)), together with the 'reciprocal boundary conditions' MD/DDD coupling method, ensure that the same dislocation segment moves at the same speed concurrently in atomistic and continuum domains [125,147,166], as shown in Figure 13(a,b). For dislocation passing, the 2D detection band is no longer used; instead, a variant of the dislocation extraction algorithm [167] is introduced to detect dislocations on the atomistic side [128], while the 'core templates' are employed to correct the linear elasticity-based displacement field on the continuum side, as shown in Figure 13(c,d). In this way, the dislocation jump distance is eliminated and a seamless two-way transmission of curved dislocation segments between the two domains is made possible [130].

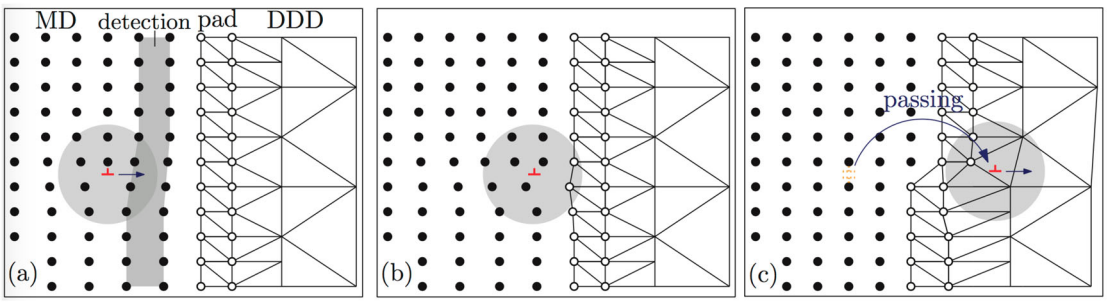

Figure 12. The procedure of the detection and passing of a dislocation across the atomistic/continuum domain interface in CADD2d. (a) An edge dislocation approaches the domain interface from the MD side, with the non-linear core region marked by the grey circle; the dislocation is detected in the detection zone. (b) Since the DDD mesh cannot sustain the highly distorted core structure, a spurious force is applied on the dislocation. (c) A dislocation dipole is introduced on the DDD side of the domain interface; the dislocation with the opposite sign with respect to the original dislocation annihilates the latter, leaving behind in the continuum domain a dislocation with the same sign as the original one. Reproduced with permission from [87].

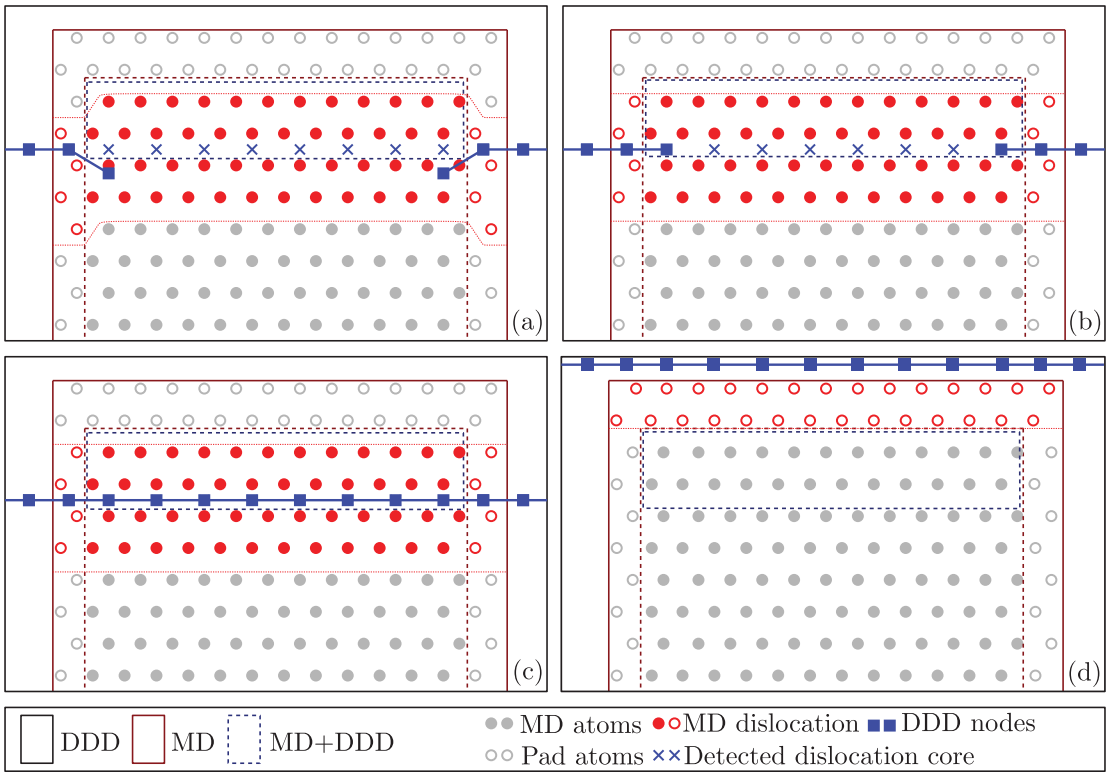

Figure 13. The procedure of the detection and passing of a straight 'hybrid' dislocation, with a short segment in the MD domain and the rest in the DDD domain, across the atomistic/continuum domain interface in CADD3d. (a–b) With the help of the 'reciprocal boundary conditions' MD/DDD coupling method, the dislocation moves toward the domain interface while remaining straight. After the dislocation is detected, new DDD nodes are introduced at the cores in the MD+DDD region in (c), followed by that all segments of the dislocation enter the DDD domain in (d). Reproduced with permission from [87].

Heat conduction

In solids, heat is transferred from one place to another via conduction, during which the heat flux is carried by vibration and movement of subatomic/microscopic particles. Among crystalline materials, the electron fluid conducts most of the heat flux in metals and some semiconductors, while phonon vibrations dominate the heat conduction in insulators and other semiconductors. In *classical* atomistics, the electrons are not explicitly accounted for while their effects are approximated by interatomic potentials. Accordingly, *classical* atomistic/continuum coupling methods can only simulate phonon-mediated heat conduction. Among the five multiscale approaches reviewed in this paper, AtC is able to simulate transports of phonons and electrons by using the two-temperature model [168], yet this capability is available only in the continuum domain, part of which always overlaps the whole atomistic domain [88]. Hence, we focus on phonon-mediated heat conduction in this section.

A collective atomic motion in crystals, phonons transport in a diffusive manner in bulk materials, and are well described by Fourier's law [169]. However, at length scales smaller than the mean free path of phonons, e.g. in nanostructures, heat flow becomes ballistic, resulting in a significant decrease in energy transport away from the heat source compared with Fourier's law predictions [170], as illustrated in Figure 14. Transport of phonons can also be classified based on its degree of coherence [171]: when atoms vibrate collectively at the same frequency with a constant phase, coherent phonons are generated; instead, when atoms vibrate randomly, which is a more common scenario in engineering materials, incoherent phonons are produced. For polyatomic crystals which have more than one atom per primitive unit cell, the vibration of atoms exhibits two different modes, namely, optical and acoustic modes, depending on whether two adjacent atoms move against each other (i.e. optical) or together (i.e. acoustic). These characteristics add to the complexity of modelling phonon-mediated heat conduction.

Experiments and simulations revealed that the characteristic length of phonons and phonon scattering events in materials with functional microstructures (e.g. superlattices and metamaterials) spans from nm to sub-mm [172,173]. Thus, phonon-mediated heat conduction is inherently a multiscale problem that falls right into the realm of atomistic/continuum coupling approaches. Similar to dislocations, the difficulty in modelling heat conduction in crystals lies in how phonons are described in the continuum domain and how

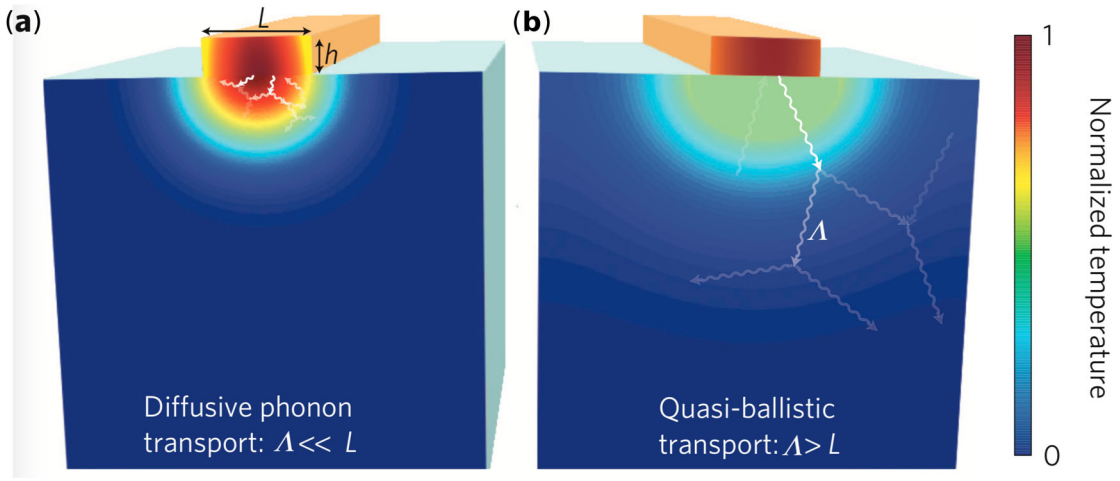

Figure 14. A schematic illustrating (a) diffusive and (b) quasi-ballistic phonon transport across a Ni/sapphire interface in experiments. The temperature field is normalised between the highest and lowest temperatures. Λ is the mean free path of the phonons in the heat sink. *L* and *h* are, respectively, width and height of the periodic Ni lines, which are in contact with a sapphire substrate. Phonons with $\Lambda = 100–150$ nm are produced by using a laser amplifier system to impulsively heat the Ni lines. Different phonon transport modes are made possible by adjusting *L* between 65 and 2000 nm. Reproduced with permission from [170].

they flow across the atomistic/continuum domain interface. Unlike dislocations which may move quasistatically, heat conduction is a non-equilibrium transport process. Therefore, in this section, we will discuss four multiscale methods – AtC, BDM, CAC, and QC – that have finite temperature non-equilibrium dynamic formulations. Note that there are two types of 'hot-QC': 'hot-QC-static' which, similar to CADD, has a static continuum domain, and 'hot-QC-dynamic' which solves the entire system dynamically [62]. As a result, 'hot-QC-static' and CADD are precluded from being applied to heat conduction. In the following, in the first subsection, we will briefly discuss these atomistic/continuum coupling methods with regard to some common challenges in their finite temperature equilibrium formulations; then, we address heat conduction in the continuum domain in the second subsection and that across the atomistic/continuum domain interface in the third subsection.

Finite temperature equilibrium dynamics

In this subsection, we discuss the first two of the three challenges in finite temperature dynamic formulations in atomistic/continuum coupling approaches as proposed in the subsection 'Finite temperature and dynamics', i.e. definition of temperature and dynamic stability, in the context of equilibrium dynamics. Unique issues encountered in non-equilibrium dynamics will be examined in the next two subsections.

Among the four multiscale methods, the temperature in the continuum domain is either directly prescribed as a thermodynamic variable (in BDM), not explicitly defined (in CAC), calculated by coupling with the atomistic domain temperature via Equation (5) (in AtC), or calculated via Equation (1) and accompanied by harmonic approximation to add the missing entropy to the kinetic energy (in QC). In CAC, on account of its applications to non-equilibrium transient phonon transport, dynamic evolution of the system is characterised by local kinetic energy instead of temperature which is well defined only in equilibrium systems [174]. For QC, based on the original static formulation [25], Shenoy et al. [61] proposed QC Monte Carlo and QC free energy minimisation methods. Dupuy et al. [81] developed another finite temperature equilibrium QC approach which employs a potential of mean force [175]. Kulkarni et al. [82] combined the variational mean-field theory and the maximum-entropy formalism to extend quasistatic QC to both equilibrium and non-equilibrium finite temperature dynamics. Later, Marian et al. [63] presented a finite temperature equilibrium extension of the QC method using Langevin dynamics. These equilibrium dynamic QC methods were summarised by Tadmor et al. [62]. Note that while quasi-harmonic approximation provides a good estimate of the entropic contribution from the thermal fluctuations of slave atoms, it is computationally intractable for most systems [62]. Hence, the local harmonic model [176] is usually adopted to simplify the calculation. Recently, Kim et al. [57] incorporated hyperdynamics [51] into 'hot-QC-dynamic' to extend accessible time scales in QC simulations. Due to the equilibrium base of the hyperdynamics, 'hyper-QC' is only applicable to equilibrium and quasi-equilibrium processes [177,178]. These equilibrium formulations are well suited to exploring temperature-dependent material properties/responses, e.g. elastic constants [61], lattice parameter [61–63,81,82], free energy [63], and nanoindentation [62,81].

Another potential issue in dynamic formulations is that the force-based methods may be dynamically unstable because they do not have a well-defined total energy. Bauman et al. [179] proposed that the Lagrange multiplier based on the L_2 norm used in BDM is unstable, yet this is not supported by other work [180,181]. Across the atomistic/continuum domain interface, the coupling scheme in dynamic BDM [46] results in an aphysical temperature gradient even in systems in mechanical and thermodynamic equilibrium. This issue was later rectified by Anciaux et al. [77] by adding a new thermostatted handshake region to the original one on the atomistic domain side. For CAC, no dynamic instability in materials at the elastic deformation stage has been observed in any prior simulation, to the best of our knowledge. Similarly, Dobson et al. [182,183] proved that the force-based QC method is dynamically stable up to the threshold of lattice defect formation.

Heat conduction in the continuum domain

When a system is out of equilibrium, the classical statements of the zeroth and second laws of thermodynamics based on equilibrium situations are ambiguous [40]. Also, terms like entropy and temperature in classical statistical mechanics become elusive [184] and may only be defined locally, as done in all four atomistic/continuum coupling methods. These aspects call for special attention to finite temperature formulations for multiscale modelling of non-equilibrium dynamic processes such as heat conduction.

The original AtC method [21] employs an energy balance equation and Fourier's law in the continuum domain to enable heat conduction. Since the atomistic domain is entirely overlaid on part of the continuum domain, this adds a drag force to the interatomic potential-based atomic force. In other words, the energy conservation is enforced by applying a thermostat force on all atoms in the atomistic domain. To let the atomistic domain evolve more freely, a modified AtC method [83] was proposed to facilitate a smooth transition between regions with different ensembles, e.g. the thermostated pseudo-NVT heat source/sink regions and the constant energy NVE region between the source and the sink. In this AtC version, constitutive equations such as Fourier's law are not needed. However, one disadvantageous ramification is that the entire continuum domain is overlaid with an atomistic domain. Consequently, a full atomistic description is required everywhere and AtC no longer extends the accessible length scale in simulations. Nevertheless, it is worth mentioning that AtC is able to couple transports of electrons and phonons and thus has the unique capability of simulating laser heating of metallic materials [88].

Similar to the original AtC method, the continuum domain of dynamic BDM [46] introduces conservation equations of mass, momentum, and energy (Equation (7)), as well as Fourier's law, except that the atomistic and continuum domains are coupled only via a small handshake region. As such, AtC and BDM are able to provide average thermodynamic states of the system, instead of the detailed effects of heat waves which are smeared out by using Fourier's law and some predefined material parameters.

On the contrary, the theoretical foundation of CAC is the Kirkwood's statistical mechanical theory of transport processes [185,186], in which the fundamental equation that links microscopic many-body dynamics $\mathbf{A}$ in the phase space to a macroscopic local density $\bar{\mathbf{A}}$ in the physical space is defined as [186]

$$\bar{\mathbf{A}}(\mathbf{x},t)=\sum_{j}^{N_a}\int_{\mathbf{r}}\int_{\mathbf{p}}\mathbf{A}(\mathbf{r},\mathbf{p})f(\mathbf{r},\mathbf{p},t)\delta(\mathbf{R}_j-\mathbf{x})\,\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{p}, \quad (17)$$

where f is a time-dependent probability function, $\mathbf{r}=\{\mathbf{R}_1,\mathbf{R}_2,\ldots,\mathbf{R}_N\}$ and $\mathbf{p}=\{m_1\dot{\mathbf{R}}_1,m_2\dot{\mathbf{R}}_2,\ldots,\ m_N\dot{\mathbf{R}}_N\}$ are a set of canonical coordinates in the phase space with $\mathbf{R}_j$ being the centre of the jth unit cell, and δ is a localisation function that relates the phase space with the physical space at the lattice level. This equation is then extended to a two-level description: lattice level continuous deformation and discrete internal deformation within individual primitive unit cells. It follows that a complete set of conservation equations, i.e. Equations (8)–(10), are derived, which, for monatomic materials, are in an identical form as the balance equations of classical continuum mechanics. These three governing equations are then supplemented by the interatomic potential to solve both continuous lattice deformation and rearrangement of atoms within unit cells. Note that for an energy-conserved system, the energy equation (Equation (10)) becomes trivial and is not needed. The fact that CAC does not introduce any empirical law maintains its predictive capability in probing structure-to-property relationships in materials at length scales much larger than those of atomistics.

In QC, as mentioned in the previous subsection, Kulkarni et al. [82] proposed the first finite temperature non-equilibrium dynamic QC method. Different from CAC which uses the Kirkwood's statistical mechanical theory of transport processes (Equation (17)), non-equilibrium QC is based on the hypothesis of local-equilibrium that follows the classical equilibrium statistical mechanics, i.e.

$$\langle\mathbf{A}\rangle=\frac{1}{N_{\mathrm{p}}!h^{3N_{\mathrm{p}}}}\int_{\mathbf{r}}\int_{\mathbf{p}}\mathbf{A}(\mathbf{r},\mathbf{p})f(\mathbf{r},\mathbf{p})\,\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{p} \quad (18)$$

where $\langle \mathbf{A} \rangle$ is a time-average observable quantity, h is the Planck's constant and the total number of particles N_p is the sum of the number of atoms in the atomistic domain and that of the slave atoms in the continuum domain. To extend this averaging scheme to a non-equilibrium system, QC employs local forms for all thermodynamic quantities. It follows that f is determined by the normalisation condition

$$\frac{1}{N_\mathrm{p}! h^{3N_\mathrm{p}}} \int_{\mathbf{r}} \int_{\mathbf{p}} f(\mathbf{r}, \mathbf{p}) \, \mathrm{d}\mathbf{r} \, \mathrm{d}\mathbf{p} = 1 \tag{19}$$

and, some local constraints applied on each particle k by Jaynes' principle of maximum entropy [187,188]: $\langle \mathbf{r}_k \rangle = \bar{\mathbf{r}}_k$ and $\langle \mathbf{p}_k \rangle = \bar{\mathbf{p}}_k$, where $\bar{\mathbf{r}}_k$ and $\bar{\mathbf{p}}_k$ are mean position and mean momentum of the kth particle, respectively. Based on f and with the help of a variational mean-field approximation, local thermodynamic potentials (entropy, internal energy, and free energy) are defined in and away from equilibrium. Local temperature T_k at the particle site k is then defined as the derivative of the internal energy with respect to the local entropy. For heat conduction, an additional discrete Fourier's law accompanied by a thermal conductivity is employed to close the system of discrete governing equations. In this way, thermo-mechanical coupling is enabled by calculating space–time temperature evolution in mechanically deformed systems.

In the meantime, the employment of mean trajectories of particles that are smooth on the time scale of thermal vibrations allows for a much larger time step than that in MD [143,189]; as a result, the length and time scales are simultaneously extended in this version of 'hot-QC' [82]. Note that this temporal coarse-graining ability naively realised in 'hot-QC' is different from that in 'hyper-QC' [57] which additionally incorporates hyperdynamics [51]; the former has both equilibrium and non-equilibrium formulations while the latter is only applicable to equilibrium and quasi-equilibrium problems, as discussed in the previous subsection. Recently, Venturini et al. [86] formulated a new discrete kinetic framework for non-equilibrium statistical thermodynamics in atomistic simulations based on kinetic equations of the Onsager type [190,191]. This new framework was introduced into the 'hot-QC' version of Kulkarni et al. [82] to yield a new finite temperature non-equilibrium dynamic QC method, which was then employed to explore nanovoid growth as will be discussed in the next subsection.

Heat conduction across the atomistic/continuum domain interface

As discussed in the subsection 'Finite temperature and dynamics', the third challenge in dynamic atomistic/continuum coupling methods is spurious wave reflection at the domain interface which mainly originates from the mismatch in vibrational mode between atomistic and continuum domains. In phonon-mediated heat conduction, this results in phonon trapping and excessive heating in the atomistic domain. Since the atomistic domain is always overlaid on the continuum domain in AtC, we only discuss phonon-mediated heat conduction across the domain interface in BDM, CAC, and QC in this subsection.

In dynamic BDM, the heat conduction across the domain interface is facilitated by the Lagrange multipliers adopted in the handshake region. In the atomistic domain, the local temperature T^M is calculated via Equation (1) in which N_p and E_kin are, respectively, the number of atoms in and kinetic energy of a 'cell' which contains several atoms, as shown in Figure 15 (a). Across the domain interface, local T^M is compared with the continuum temperature T^C in the handshake region, thus transferring heat along the direction dictated by the second law of thermodynamics. While the two-way exchange of heat between two domains is relatively smooth (Figure 15(b,c)), spurious wave reflections still exist. To overcome this problem, Sadeghirad and Tabarraei [84], Sadeghirad and Liu [192], and Tabarraei et al. [193] decomposed the displacement field of the atoms in the handshake region into a mechanical wave-induced coarse field and a thermal vibrations-induced fine field, followed by that the fine component is damped using local thermostats. Validation of this new coupling scheme was achieved by realizing smooth heat conduction along a 1D rod.

In dynamic CAC, transports of medium ($\approx$ 15.34 nm) and long ($\approx$ 51.12 nm) wavelength phonons from the atomistic domain to the continuum domain in a 1D rod were simulated [85]. It is found that in polyatomic crystals with up to three atoms per primitive unit cell, complete branches of these phonons are transmitted across the domain interface; as a result, the continuum domain in CAC, albeit predicting a larger phonon wavelength [91], is identical to MD from the perspective of kinetic energy conservation. Recently, an atomic-vibration-based coherent phonon pulse model [194] has been incorporated into CAC to simulate medium to long-wavelength (5–250 nm) ballistic-diffusive phonon heat transport across Σ19 symmetric tilt grain boundaries (GBs) in Cu [92]. As shown in Figure 16, the phonon pulse propagation across the GBs (rendered in atomistic resolution) is partially ballistic and partially diffusive, with the ballistic phonons coherently transported across while most of the energy carried by the diffusive phonons impeded by GBs; also, the phonon/GB interactions alter local GB structures. Nevertheless, the phonon dispersion relations in the atomistic and continuum domains overlap with each other only for wavelengths that are larger than a certain value [120]; in other words, the spurious wave reflections persist if short-wavelength phonons are

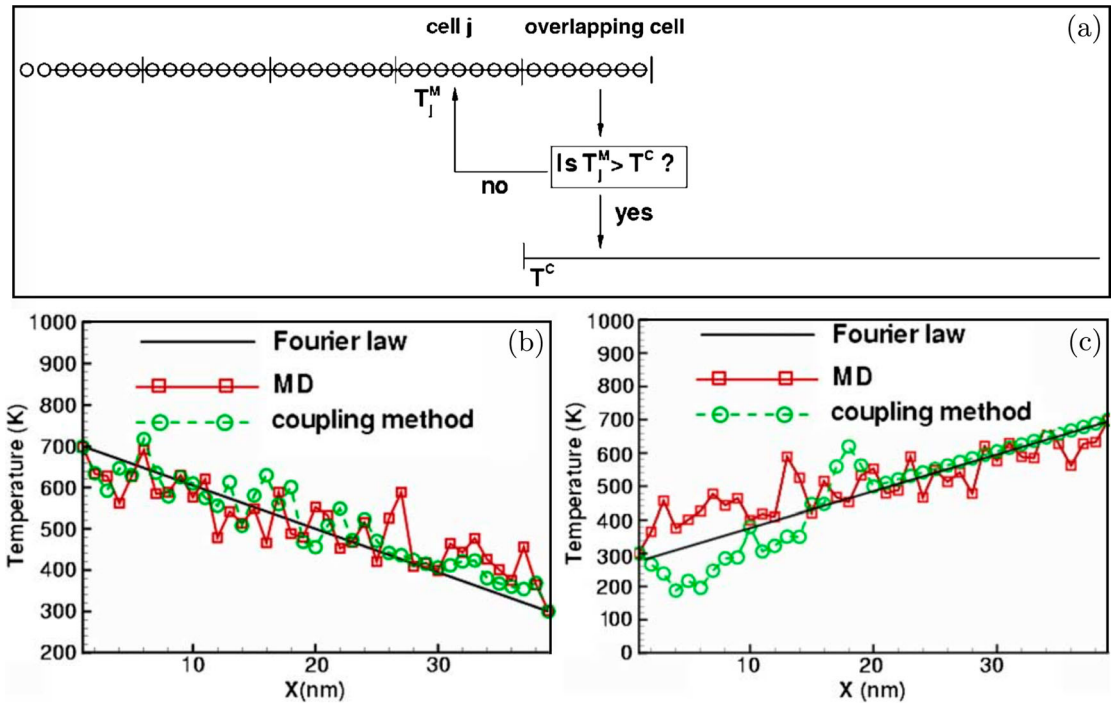

Figure 15. (a) 1D schematic of a BDM model for heat conduction from the atomistic domain to the continuum domain; the atomistic domain is divided into cells, the rightmost of which overlaps the left end of the continuum domain. (b) and (c) are comparisons of the temperature distribution in a 1D steady state system predicted by the coupling method (i.e. BDM), MD, and Fourier's law, respectively. In (b), a heat source is in the atomistic domain while a heat sink is in the continuum domain; it is vice versa in (c). Reproduced with permission from [46].

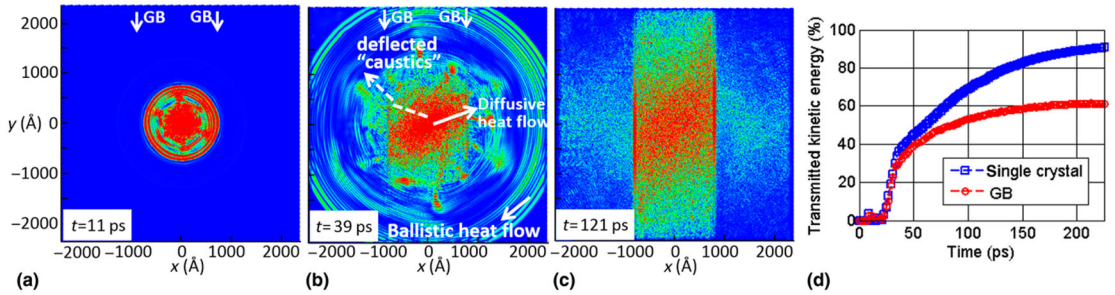

Figure 16. (a–c) Kinetic energy evolution shows the transient phonon heat propagation across two Σ19 symmetric tilt GBs in Cu. The GBs are located in two separate atomistic domains. The kinetic energy field is normalised between the highest and lowest kinetic energy. (d) The transmitted kinetic energy across GB quantifies the resistance of the GB to phonon heat transport. Reproduced with permission from [120].

included. To address this problem, instead of trying to eliminate or damp out short wavelength phonons as in BDM [84,192,193], the ultimate goal of CAC is to pass full-spectrum phonons across the domain interface. Recently, a first attempt has been made to employ a 1D wave-based finite element shape function to permit a two-way passage of short wavelength (2.51 nm), high-frequency phonon waves between atomistic and continuum domains [93]. However, this novel shape function is still at the proof-of-concept stage and has not yet been extended to 2D and 3D.

In non-equilibrium 'hot-QC' [82,86], an average thermodynamic behaviour is obtained by introducing a variational mean-field approximation, as discussed in the previous subsection, to eliminate thermal vibrations from the dynamics. Thus, spurious wave reflections at the atomistic/continuum domain interface are likewise mitigated [143]. In recent years, non-equilibrium 'hot-QC' simulations have been carried out in metallic materials to investigate 3D nanovoid growth, with an atomistic domain resolved in the vicinity of the nanovoid while the continuum domain is used elsewhere. For example, the 'hot-QC' method of Kulkarni et al. [82] was employed to simulate nanovoid growth in Cu [142], which found that the critical tensile pressure for initial dislocation nucleation from void surface is approximately temperature-independent at low temperatures but decreases steadily

when the temperature is higher than 250 K, indicative of strong thermal activation. Later, the 'hot-QC' method modified based on the work of Venturini et al. [86] was adopted to explore nanovoid growth in Cu [143,145], Al [145], and Mg [144]. A wide range of strain rates between 10^5 and 10^{10} s^{-1} were used to probe the strain rate effect on nanovoid cavitation, revealing a strong and complex interplay among strain rate, temperature, and plasticity in materials. As shown in Figure 17, a transitional strain rate on the order of 10^7 s^{-1} is identified: at low strain rates, the voided system remains nearly isothermal with low dislocation velocities; at high strain rates, the behaviour of the material becomes adiabatic, accompanied by high dislocation velocities.

Dislocation/phonon interactions in the continuum domain

In crystalline materials, a moving dislocation is resisted by intrinsic and extrinsic barriers as well as drag processes, the last of which arise from its interaction with various elemental excitations in crystals such as phonons and electrons [195]. In an otherwise perfect lattice with a low Peierls barrier, the scattering of phonons by dislocations is the primary source of the damping of dislocation motion [196]. Recently, Li et al. [197] proposed to treat a dislocation line as a quantised field to consider both vibrating dislocation line and long-range strain field, as shown in Figure 18. In the meantime, as the dislocation moves in a discrete lattice, its core structure changes periodically, inducing radiation friction to dislocation motion and affecting thermal properties of the material by emitting new phonons [198]. As such, interactions between dislocations and phonons are extremely complicated and their simulation is one of the grand challenges in modelling phonon transport in materials [199]. While atomistic methods such as MD allow direct assessment of phonon emission and scattering by dislocations, long-wavelength phonons and dislocation elastic field as well as long-distance travel of dislocations are beyond their accessibility [200,201]. At the mesoscale, on the one hand, DDD and phase field methods [202] have gained wide popularity in modelling dislocations; on the other hand, the Boltzmann transport equation for the motion of phonons in solids [203] may be numerically solved via XFEM [204]. Thus, it is conceptually possible to simultaneously resolve dislocations and phonons using XFEM. However, we are not aware of any research effort in this direction. More generally, it is not clear how dislocations and phonons may be simulated in the same continuum-level framework. Given the characteristic nm length scale of a dislocation core and much longer range of elastic waves of phonons, dislocation/phonon interactions are patently multiscale. Among the five atomistic/continuum coupling methods reviewed in this paper, only CAC has been applied to dislocation/phonon interactions, to the best of our knowledge.

Xiong et al. [89] found that the sub-THz phonon drag coefficient in dislocation/phonon interactions increases with incoming phonon wave packet magnitudes or sizes but is insensitive to the incident angles. Later, Xiong et al. [91] discovered that a fast moving dislocation has a velocity-dependent asymmetric stress field in which the leading partial dislocation possesses a higher stress level than the trailing partial dislocation as a result of the emitted phonon waves. More recently, motivated by the ultrafast heat pulse experimental technique used in thermal measurements of materials at the nano to mesoscale [205,206], the development of dynamic CAC focused on simulating phonon pulse propagation and its interaction with lattice

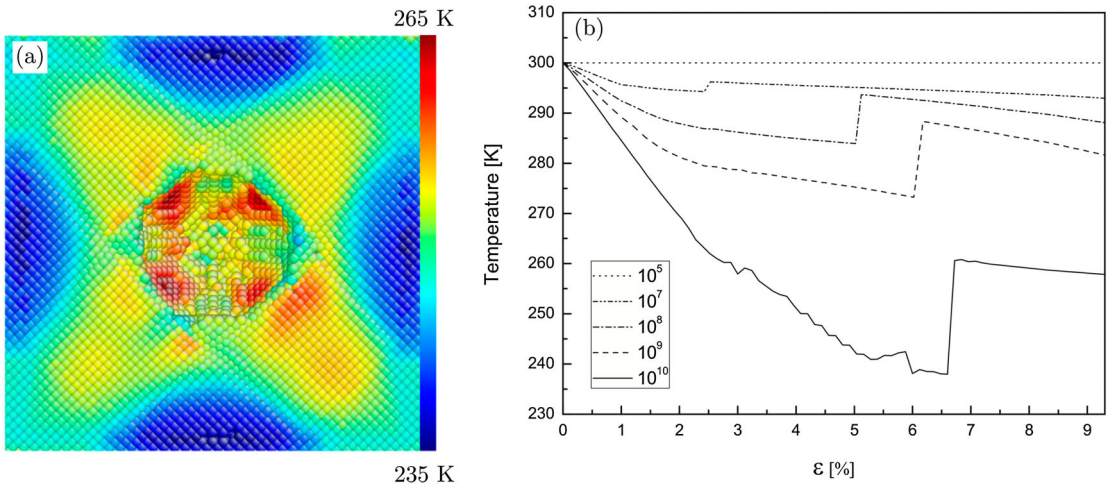

Figure 17. (a) Temperature field near a spherical nanovoid in a Cu single crystal that is subject to volumetric tensile deformation at a strain rate of 10^{10} s^{-1} recorded at 7.3% strain; the initial temperature for the undeformed system was 300 K; (b) Temperature evolution near the surface of the nanovoid at different strain rates in units of s^{-1}. Reproduced with permission from [143].

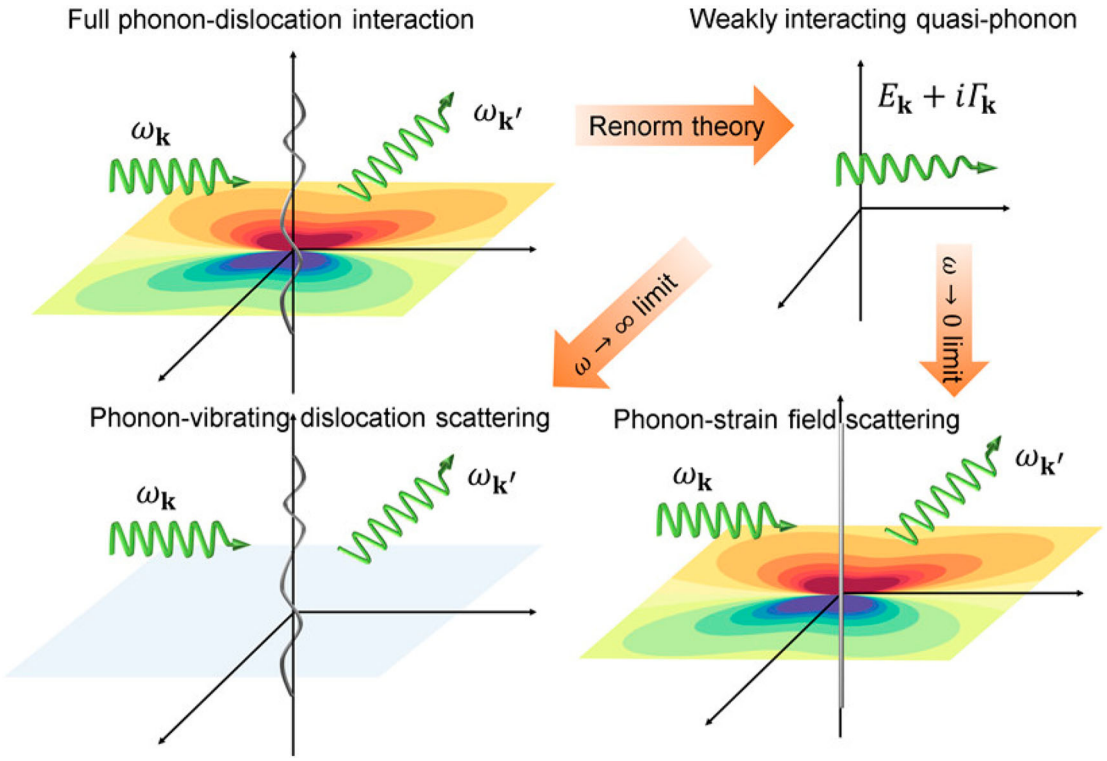

Figure 18. The quantum picture of the interactions between a phonon with frequency $\omega_{\mathbf{k}}$ and a vibrating dislocation based on the renormalisation (renorm) theory. By treating a dislocation line as a quantised field, the dislocation/phonon interaction results in a weakly interacting quasi-phonon with a renormalised energy $E_{\mathbf{k}}$ and a finite lifetime $\Gamma_{\mathbf{k}}$. When $\omega_{\mathbf{k}}$, respectively, approaches ∞ and 0, the renorm theory reduces to classical theories of phonon/vibrating dislocation scattering and phonon/strain field scattering, with the emission of a new phonon with frequency $\omega_{\mathbf{k}'}$. Reproduced with permission from [197].

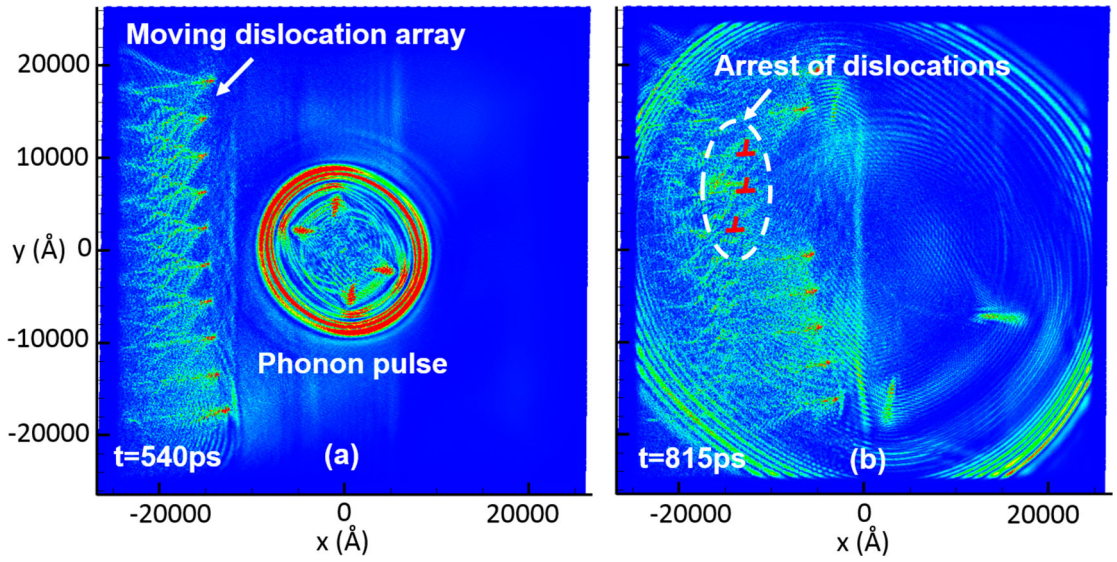

Figure 19. Time history of the kinetic energy distribution showing dislocations arrested by phonon pulse propagation in a Cu single crystal with uniformly sized finite elements. Finite element nodes are coloured in the same way as in Figure 16. Reproduced with permission from [94].

defects such as GBs and dislocations. Chen et al. [94] studied a coherent phonon pulse interacting with multiple moving dislocations and reported that phonons lower the energy associated with the moving dislocation cores, with some energy lagging behind the decelerated dislocation or dispersed around the arrested dislocation through the emission of secondary phonon waves, as shown in Figure 19. We remark that the discrepancies in the dynamic continuum domain with respect to MD, such as a higher dislocation mobility [91], result in coarse-graining errors in CAC-predicted dislocation/phonon interactions.

Conclusions

The field of multiscale materials modelling using atomistic/continuum coupling approaches saw explosive development since the first method of this kind was proposed in 1991 [29]. Much effort has been devoted to methodological development, with a focus on enriching the physics in the continuum domain to represent defects and heat as well as increasing the fidelity of information passing across the atomistic/continuum domain interface [14]. Recently, there was an emerging trend in the community towards applying these elegant and sophisticated multiscale methods to solving important material problems in engineering. To echo this exciting research direction, in this paper, we review five representative atomistic/continuum coupling techniques that were actively being developed in the last decade, including AtC, BDM, CAC, CADD, and QC, in a problem-centric manner. We aim at clarifying how each method simulates dislocations and phonon-mediated heat conduction as well as the more complicated dislocation/phonon interactions in crystalline materials.

We first discuss the strengths and limitations of atomistic/continuum coupling methods in general, as well as three common outstanding challenges in their development, including statics, finite temperature and dynamics, and mesh refinement. Then, we provide a brief discussion of key characteristics of the five multiscale approaches, which are summarised in Table 1. Further discussions of the five methods are focused on their applications to dislocation, heat conduction, and dislocation/phonon interactions. The main conclusions are:

(1) CAC [23] and CADD [24], via, respectively, employing discontinuous finite elements and DDD in their continuum domains, enable a two-way exchange of dislocations between the atomistic and continuum domains, while the other three methods do not permit dislocations in the continuum. Both CAC and CADD have been extended to 3D in which curved dislocation segments can be transferred across the atomistic/continuum domain interface. Note that in the current form of XFEM-BDM [95,96], a large portion of the slipped region, but not the dislocation itself, is solved by XFEM in the continuum domain; yet XFEM-BDM may be modified to realise the two-way exchange of dislocations by incorporating the core enrichment function [155] into XFEM. Accordingly, we review dislocations in the continuum domain in XFEM-BDM, CAC, and CADD and conservative dislocation movement on the same slip plane across the domain interface in CAC and CADD.

(2) AtC [21], dynamic BDM [46], dynamic CAC [85], and 'hot-QC-dynamic' [82,86] are equipped with finite temperature non-equilibrium dynamic formulations and are thus applicable to non-equilibrium processes such as heat conduction. By comparison, similar to 'hot-QC-static' [62], dynamic CADD [79] combines a dynamic atomistic domain with a quasistatic continuum domain, with a damping band to eliminate phonon waves; as a result, 'hot-QC-static' and CADD are precluded from being applied to heat conduction. Among the four capable multiscale techniques, AtC is able to simultaneously model transports of phonons and electrons while the other three methods can only simulate phonon-mediated heat conduction; 'hot-QC-dynamic' employs local forms of thermodynamic quantities and a mean-field approximation to obtain an average thermodynamic behaviour with relatively small thermal fluctuations; CAC focuses on phonon-mediated heat conduction, with its theoretical foundation on non-equilibrium statistical mechanical theory for transport processes and its goal of complementing MD by providing missing long-wavelength phonon information. In this context, we discuss finite temperature equilibrium dynamics as well as issues raised by nonequilibrium dynamics such as heat conduction in the continuum domain and heat conduction across the domain interface.

(3) Lastly, for the more complicated problem of dislocation/phonon interactions, we review recent progresses of the CAC method in this direction, as CAC is the only approach among the five that can resolve both dislocations and phonons in the continuum domain. Preliminary CAC simulations [89,94] showcase the complexity of space and time-evolving of fast moving dislocations and lattice waves, as well as their interactions.

Challenges and perspectives

The ultimate goal of developing and applying atomistic/continuum coupling approaches is to combine atomic-level accuracy with macroscale efficiency in solving material problems in engineering. By complementing nano/microscale experiments [207,208], these state-of-the-art multiscale materials modelling methods have the potential to provide enhanced reliability in linking processing, structure, property, and performance on the length and time scales necessary for discovery, design, development, and deployment of novel materials for the future. Key tasks ahead involve both methodologies and applications, which should progress hand in hand. The present

review of the capabilities, difficulties, and effectiveness of the applications of the five multiscale methods to the modelling of dislocations and heat conduction in crystalline materials calls for attention to the following three areas: advanced atomistic modelling, enrichment of the physics in the continuum, and high-fidelity information passing across the domain interface. Advances in these areas will facilitate the applications of the atomistic/continuum coupling methods to a broader variety of important engineering problems; some specific suggestions are as follows:

(1) As mentioned in the section 'Heat conduction', in *classical* atomistics, the electrons and chemical bonds are not explicitly described. While this facilitates capturing main atomic-level materials properties/responses, phenomena that require explicit modelling of electrons and bonds are grossly approximated. For example, in metals, the heat conduction is dominated by the electron fluid; also, for a dislocation that is moving at low temperatures, the electron drag may be more pronounced than the phonon drag [195]. Another example is the chemical reactions during which bonds frequently break and form. To realise full thermo-electro-chemo-mechanical-coupling, especially for functional materials, (i) advanced atomistic approaches may be used to explicitly account for electron transport [209,210] and (ii) reactive interatomic potentials such as the reactive force field [211,212] and the charge optimised many-body potential [213] may be employed.

(2) The enrichment of the physics in the continuum demands developing advanced continuum-level theories for more general lattice defects, e.g. point defects, GBs, and cracks, as well as their interactions in the presence of heat waves, such that the size of the atomistic domain can be further reduced. Another tangible but not straightforward task is to integrate the temporal coarse-graining methods that have been implemented in atomistic simulations into the continuum domain to access an extended period of time involved in processes such as diffusion, creep, and corrosion. For example, the transition state theory-based techniques [214] such as the nudged elastic band method [50] would allow the multi-length scale methods to probe the energy barrier and more sophisticated minimum energy pathway for extended microstructures at the submicron and micron scales that are not accessible by accelerated MD. Some efforts in this direction have been made for the coarse-grained MD method [215,216] and DDD [217], but not for any of the five multiscale approaches reviewed in this paper, to the best of our knowledge.

(3) Usually, it is not critical to pursue an exact description of defects and heat in the continuum domain if the essential defects interactions take place in a region in the atomistic domain away from the domain interface. In other words, as long as the necessary information is passed into the atomistic domain, the simulation results are trustworthy. Therefore, the validity of an atomistic/continuum coupling method heavily hinges on the fidelity of the information flow across the domain interface, more so for the one from an atomistic domain to a continuum domain than the other way around, owing to the more DOFs in atomistics. Take the short-wavelength phonons as an example, they are either passed into the continuum domain via overlaying the whole atomistic domain (in AtC [21]), employing an enriched finite element shape function (in dynamic CAC [93]), averaging the thermodynamic behaviours in the continuum (in 'hot-QC-dynamic' [82]), or damped out by a damping band on the atomistic side of the interface (in dynamic BDM [84] and dynamic CADD [47]). More scientific pursuits in this regard with advanced high-performance computing techniques are warranted.

Despite being a powerful tool to potentially bridge the traditional gap between experiments and atomistic-based simulations, atomistic/continuum coupling approaches to date have been mostly applied to relatively simple and small-scale unit processes that are of scientific interests. In our opinion, this is mainly because (i) these methods are at an early development stage with respect to the complexity of real engineering problems and (ii) the applications of these methods at large length/time scales are intrinsically compute-intensive. In terms of the material types, many engineering materials such as alloys and composite materials [218] are multi-constitute and/or polyatomic, the latter of which is more challenging in the continuum domain from the perspective of modelling because simple finite element shape functions may not hold. To date, multiscale simulations based on BDM [181], CAC [59,85,114–116,219], and QC [220–222] have been carried out to investigate polyatomic crystalline materials. Efforts have also been made to develop coarse-grained atomistic methods for non-crystalline materials [223–225]. However, it is challenging to employ atomistic/continuum coupling methods to explore complex materials and processes such as metal/polymer composites, organic/inorganic composites, and droplet/surface interactions in additively manufactured microfluidic devices. Future work in this direction may offer hope to aiding a wider range of engineering applications.

Nevertheless, existing multiscale methods for relatively simple crystals can be applied to some important engineering problems to produce new materials science

knowledge. For example, one of the grand challenges of the new era of simulation-assisted discovery and design of new materials is the prediction of the interactions of dislocations with grain and phase boundaries [10]. This topic has been explored using CAC [76,118], CADD [131,132,134], and QC [226–231]. A related topic – crack/GB interactions – has also been pursued in simulations based on CAC [59] and QC [226,232,233]. Still, more general dislocation/crack types with different curvatures interacting with more general GBs need to be considered if researchers were to fully understand polycrystal plasticity.

Acknowledgments

The authors thank Dr David L. McDowell, Dr Youping Chen, Dr Liming Xiong, Dr Jinghong Fan, Dr Robert Gracie, Dr Shaoping Xiao, Dr Jaehyun Cho, Dr Saeed Zare Chavoshi, and Dr Marat Latypov for helpful discussions.

Disclosure statement

No potential conflict of interest was reported by the authors.

Funding

The work of SX was supported in part by the Elings Prize Fellowship in Science offered by the California NanoSystems Institute (CNSI) on the UC Santa Barbara campus. SX also acknowledges support from the Center for Scientific Computing from the CNSI, MRL: an National Science Foundation (NSF) MRSEC (DMR-1121053). The work of XC was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Division of Materials Sciences and Engineering under Award # DE-SC0006539. This work used the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation [grant number ACI-1053575].

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