# Thermal Fluctuations as a Computational Microscope for Studying Crystalline Interfaces: A Mechanistic Perspective

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*Interfaces such as grain boundaries are ubiquitous in crystalline materials and have provided a fertile area of research over decades. Their importance stems from the numerous critical phenomena associated with them, such as grain boundary sliding, migration, and interaction with other defects, that govern the mechanical properties of materials. Although these crystalline interfaces exhibit small out-of-plane fluctuations, statistical thermodynamics of membranes has been effectively used to extract relevant physical quantities such as the interface free energy, grain boundary stiffness, and interfacial mobility. In this perspective, we advance the viewpoint that thermal fluctuations of crystalline interfaces can serve as a computational microscope for gaining insights into the thermodynamic and kinetic properties of grain boundaries and present a rich source of future study.* [DOI: 10.1115/1.4037885]

*Keywords: thermal fluctuations, molecular dynamics, grain boundaries, statistical mechanics*

## 1 Introduction

Imagine a two-dimensional (2D) fluid or solid membrane[2] in thermal equilibrium. Macroscopically, the membrane may appear to be flat or smooth, but it exhibits undulations on the microscopic scale that stem from the thermal oscillations of the constituent atoms and molecules. How large these thermal effects are depends on intrinsic material properties, and is related to the energy contributions from different mechanisms causing the perturbation, namely, out-of-plane bending and in-plane stretching (areal change to accommodate the out-of-plane curving) of the membrane [1–3]. In the case of fluid membranes such as biological membranes, the bending elastic energy makes the dominant contribution, whereas in the case of solid crystalline membranes like graphene, the bending and in-plane deformation modes are coupled.

At absolute zero temperature, the equilibrium configuration is the perfectly flat membrane which is obtained by minimization of the energy consisting of the bending energy and surface tension contributions. However, at nonzero temperature, there is a finite probability of finding the membrane away from the perfectly flat configuration given by the Boltzmann formula [4]

$$p_i \propto \exp\left(-E_i/k_BT\right) \tag{1}$$

Here, $p_i$ is the probability of the $i$th mode, $E_i$ is the associated energy, $k_B$ is the Boltzmann constant, and $T$ is the temperature. Knowing the probability distribution then furnishes a complete statistical description of the fluctuating membrane and enables us to gain simplified yet valuable quantitative insights into macroscopic properties that emerge from the underlying complex nature of the membranes. The statistical mechanics of membranes has been successfully applied and extended to extract important physical parameters, such as the bending modulus and surface tension, and understand a host of phenomena associated with 2D materials that can have tremendous physiological and technological applications. These include the steric interaction between biological membranes, their electromechanical coupling, entropic effects on the morphology of crystalline membranes, and edge effects to name a few [5–10].

We find it fascinating that the statistical mechanics of free-standing membranes even applies beautifully to grain boundaries embedded in three-dimensional solids. A simple notion that interfaces are essentially two-dimensional membranes separating different phases permits us to isolate the interface or grain boundary from the bulk phases and study its out-of-plane thermal fluctuations by assigning an appropriate interfacial energy. Perhaps, it is not surprising that interfaces in crystalline solids exhibit extremely small out-of-plane fluctuations, with amplitudes on the order of a mere few nanometers and time-periods on the order of a few picoseconds. This begs the question whether the study of these fluctuations might well be an exercise in futility. Our goal here is to convince the reader that it is quite the contrary!

In fact, the statistical mechanics of fluctuating interfaces provides an attractive means to characterize grain boundaries, interphase boundaries, and crystal-melt interfaces that play a vital role in microstructural evolution, and hence in engineering materials for various applications. It is fortuitous that the spatio-temporal scale of the interfacial fluctuations, albeit small, makes them perfectly suited for monitoring via atomistic methods such as molecular dynamics simulations. This furnishes a convenient window of opportunity to probe these equilibrium fluctuations and extract various important physical parameters. Statistical mechanics, and in particular, the celebrated fluctuation–dissipation relation, have enabled the theoretical analysis of the thermal fluctuations of interfaces for decades to gain mechanistic insights into both their equilibrium and nonequilibrium properties. Now, complemented by large-scale atomistic simulations, they provide an even more unique and efficient framework for a comprehensive investigation of the mechanical behavior of crystalline interfaces to ultimately predict the overall macroscopic material response.

In Secs. 2–4, we present a few select methods that have enabled fresh insights into interfacial characteristics based on thermal fluctuations. We demonstrate the use of statistical mechanics of

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[2]By the term "membrane," we follow the physics literature and understand it to mean a two-dimensional elastic sheet that is flexible.

Contributed by the Applied Mechanics Division of ASME for publication in the Journal of Applied Mechanics. Manuscript received September 5, 2017; final manuscript received September 8, 2017; published online September 22, 2017. Editor: Yonggang Huang.

  

interfaces to obtain key parameters such as grain boundary free energy and stiffness, and to treat fluctuating interfaces as Brownian particles to compute their mobilities. We hope that they provide compelling evidence to support our viewpoint that thermal fluctuations of crystalline interfaces can indeed serve as a computational microscope for gaining insights into their thermodynamic and kinetic properties and present a rich source of future study.

## 2 Crystalline Interfaces as Fluctuating Elastic Membranes

There is a rich literature on the statistical thermodynamics of membranes which was primarily developed for soft materials—fluid and polymerized membranes—that exhibit large fluctuations (see monographs by Safran [1] and Nelson et al. [2]). In recent years, the membrane theory has also been applied and extended to study crystalline membranes such as graphene and other two-dimensional materials [11–13], as well as crystalline interfaces, such as grain boundaries, and solid–liquid interfaces [14–16] based on thermal fluctuations. In particular, we refer the reader to Refs. [11] and [13] for nice, concise reviews of these applications.

In the case of solid–solid or solid–liquid interfaces, the central idea is that the energetic cost for the out-of-plane deformation of the interface, which naturally involves deformation of the adjoining bulk regions, is used to construct an energy associated only with the interface. Then, the surrounding bulk is ignored, and the interface is regarded as a membrane with an appropriate interfacial energy.

To obtain the fluctuation spectrum of an interface, we treat the interface as a quasi-one-dimensional or ribbon-like membrane that is thin in one direction so that the fluctuations along that axis can be ignored (Figs. 1 and 2). As seen in Fig. 2, let $b$ be the width along the $z$-direction, $W$ be the length along the $x$-direction, and $h(x)$ be the out-of-plane displacement or height of the interface. Assuming that the height fluctuations are small in amplitude ($h_x \ll 1$ where $h_x \equiv dh/dx$), the energy cost for the fluctuation of the interface is [14]

$$E = \frac{1}{2} b\,\Gamma \int_0^W h_x^2\, dx \tag{2}$$

which penalizes an increase in area due to curving of the interface. Here, $\Gamma$ denotes the interfacial stiffness and is analogous to the surface tension in membrane theory. $\Gamma = \gamma + \gamma''$ is derived as the sum of the interface free energy $\gamma$ and its second derivative with respect to the orientation of the interface normal given by $h_x$. Assuming periodic boundary conditions, we can expand $h(x)$ in Fourier space as

$$h(x) = \sum_k A(k) e^{ikx} \tag{3}$$

Invoking the equipartition of energy from statistical mechanics due to the quadratic form of the energy in Eq. (2), we obtain the relationship between the mean square fluctuation spectrum and the wave number

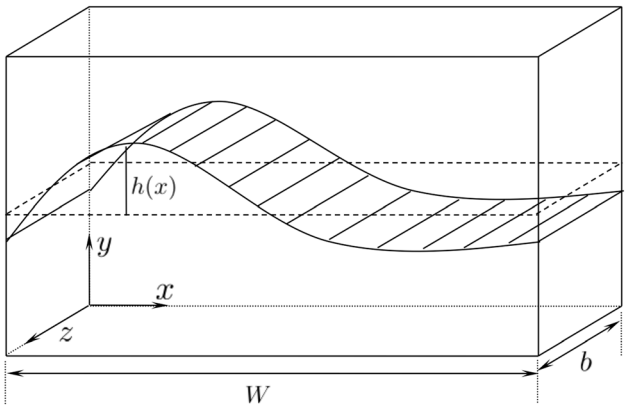


**Fig. 2 Schematic of a bicrystal representing the flat interface by dotted lines and the fluctuating interface at finite temperature by solid lines**

$$\langle |A(k)|^2 \rangle = \frac{k_B T}{bW\Gamma k^2} \tag{4}$$

where $\langle \cdot \rangle$ represents ensemble average. Equation (4) demonstrates that the fluctuation spectra generated from molecular dynamics simulations can be exploited to compute the grain boundary or interfacial stiffness, $\Gamma$, as well as the interface free energy, $\gamma$. The dependence of these parameters on temperature and grain boundary misorientation can also be comprehensively investigated. Previous atomistic studies have shown that the fluctuations of high angle grain boundaries and solid–liquid interfaces in face-centered-cubic metals indeed follow Eq. (4) [14,15]. In membrane theory, thermal fluctuations that follow Eq. (4), implying that they are accommodated by an increase in the membrane area, are also known as capillary fluctuations.

However, not all grain boundaries exhibit capillarity induced fluctuations. A recent study by Karma et al. [21] revealed that the fluctuations of boundaries that undergo shear-coupled normal motion, such as many low-angle grain boundaries, display a significantly different response. Shear-coupled motion refers to the motion of a grain boundary normal to the boundary plane when subjected to shear deformation parallel to the boundary plane. For these boundaries, the energetic cost for out-of-plane perturbation arises from the localized shearing of the crystal lattices in opposite directions at the peaks and troughs of the perturbed profile of the grain boundary. Based on this characteristic, a modified expression for the fluctuation spectrum of shear-coupled grain boundaries can be derived [21]

$$\langle |A(k)|^2 \rangle = \frac{k_B T}{bWC\beta^2 k} \tag{5}$$

Here, $C$ is a parameter comprising the elastic constants of the materials, and $\beta$ is a coupling factor defined as $\beta = v_{||}/v_n$. Introduced by Cahn et al. [22], $\beta$ characterizes the coupling relationship between the velocity parallel to the grain boundary ($v_{||}$) and the concomitant normal grain boundary velocity ($v_n$) during

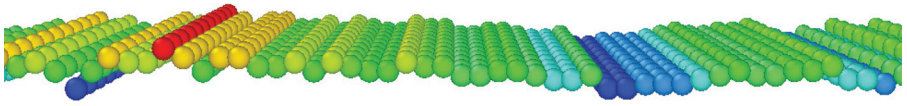

**Fig. 1 Atomistic configuration of a fluctuating coherent twin boundary in a face-centered cubic metal obtained from molecular dynamics. The colors represent the distance of the atoms above (red) and below (blue) the initial flat configuration. The fluctuations have been exaggerated for illustration. The simulations were performed in LAMMPS [17] using the embedded-atom method (EAM) interatomic potential developed by Mishin et al. [18] for Cu and visualized in OVITO [19]. Reproduced from Chen and Kulkarni [20].**

shear-coupled motion. Chen and Kulkarni [20] showed that coherent twin boundaries also follow this behavior (Eq. (5)) since they exhibit shear-coupled normal motion up to near the melting temperature.

It is interesting that although Eqs. (4) and (5) reveal different relationships between their fluctuation spectra $\langle |A(k)|^2 \rangle$ and the wave number $k$, they essentially follow a power law with different exponents for $k$. Figure 3 shows the fluctuation spectra for $\Sigma5(310)$ grain boundary and $\Sigma3(111)$ coherent twin boundary which display $1/k^2$ and $1/k$ response, respectively. Thus, treating the crystalline interfaces as fluctuating elastic membranes furnishes an effective method for computing properties such as the interfacial stiffness, and free energy as well as identifying the grain boundary characteristics simply based on their fluctuating spectra extracted from molecular dynamics simulations.

## 3 Crystalline Interfaces as Brownian Particles

Interface mobility is a key parameter in governing interfacial kinetics. Taking into account the structural dependence and environment factors, the mobility is an intrinsic property of the interfaces that dictates the motion of interfaces, and hence, microstructural evolution. Under equilibrium conditions, the interface mobility $M$, is the proportionality coefficient relating the exerted pressure $F$ and the migration or normal velocity of the interface $v$

$$v = MF \tag{6}$$

Exploiting this linear relation, several methods have been developed to estimate the mobility of interfaces using various driving forces including interfacial curvature, and applied elastic and plastic strains. These computations are performed under large driving forces far from equilibrium (and often far from the physical reality). Based on the thermal fluctuations of interfaces, Trautt et al. [16] introduced a novel computational method, the so-called interface random walk method, to capture the interface mobility in the zero driving force limit. The approach is based on monitoring the motion of the mean position of the interface which happens to be a random walk along the direction normal to the (flat) interface. The fluctuation–dissipation relation is then invoked to relate the diffusion coefficient associated with this Brownian motion with the interface mobility.

Consider a fluctuating interface under periodic boundary conditions with $\mathbf{r}(x, z)$ representing the in-plane position coordinate and $h(t)$ denoting the interface height profile at time $t$ (Fig. 4). The central idea is that for a fluctuating interface, the driving force in Eq. (6) includes the capillary force, $f_c(\mathbf{r}, t)$, and the thermal noise expressed as a Langevin force $\xi(\mathbf{r}, t)$. Then, Eq. (6) becomes

$$v = \frac{\partial h(\mathbf{r}, t)}{\partial t} = M\left[f_c(\mathbf{r}, t) + \xi(\mathbf{r}, t)\right] \tag{7}$$

where the capillary force acts like a curvature restoring force and is simply the interfacial stiffness multiplied by the curvature, that is, $f_c = \Gamma(h_{xx} + h_{zz})$ using the small slope approximation ($h_x \ll 1$, $h_z \ll 1$). The thermal noise $\xi(\mathbf{r}, t)$ is uncorrelated in space and time. Integrating this relation in space and time furnishes the interface "diffusion equation" in terms of the variance $\langle \bar{h}^2(t) \rangle$

$$\langle \bar{h}^2(t) \rangle = \frac{2Mk_BT}{A} t \tag{8}$$

where $A$ is the area of the flat interface, and $D = 2Mk_BT/A$ is the diffusion coefficient. $\bar{h}(t)$ denotes the mean boundary displacement which is calculated as the average displacement of every atom residing in the interface in the direction of migration at time $t$.

Note that this fluctuation–dissipation relation for an interface is analogous to the diffusion equation for a particle exhibiting Brownian motion. Thus, the method shows that the average interface position may be regarded as a Brownian particle performing a random walk in the direction normal to the interface plane. This provides an efficient way to estimate the mobility from atomistic simulations. As an example, Fig. 5 shows the temporal evolution of the variance $\langle \bar{h}^2 \rangle$ for the $\Sigma17(410)$ grain boundary in Ni at 1200 K. The mobility of the interface can be computed from the slope of the curve. Furthermore, for an interface performing Brownian motion, the probability of finding the average interface position should follow a Gaussian distribution centered at the initial position ($\bar{h}(0) = 0$) which becomes broader with time [4]. This is beautifully confirmed by molecular dynamics simulations as shown in Fig. 6.

Since the out of plane fluctuations are small, the interface random walk method is effective at very high temperatures, usually above 0.8 homologous temperature, which hampers its application

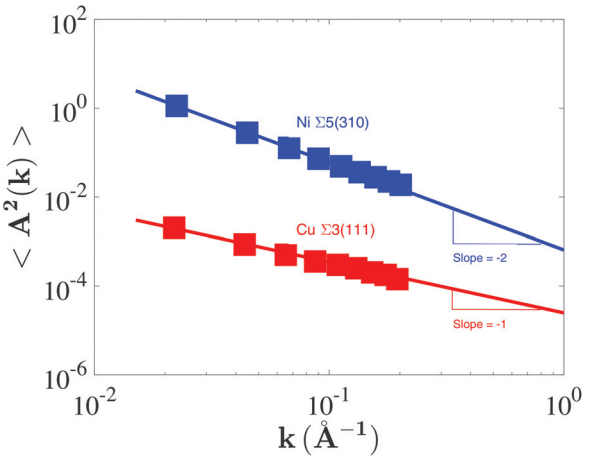


**Fig. 3 Power spectra of the thermal fluctuations of two interfaces as a function of wave number *k* obtained by molecular dynamics simulations. The red points represent Σ3(111) twin boundary with a slope of −1 (shown by a solid line). The blue points represent Σ5(310) high angle grain boundary with a slope of −2 (shown by a solid line). The simulations were performed in LAMMPS [17] using the EAM interatomic potential developed by Mishin et al. [18] for Cu and by Ackland et al. [23] for Ni.**

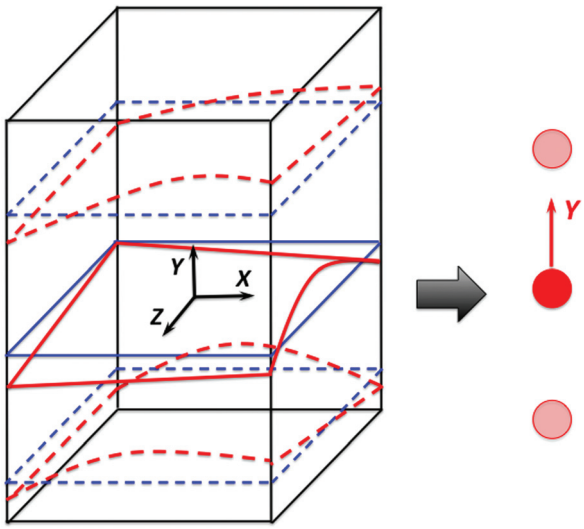


**Fig. 4 A schematic of a grain boundary fluctuating from the equilibrium position (indicated by the solid red line) to new positions (indicated by the dashed red lines). The random walk of the mean grain boundary positions (indicated by the dashed lines) deviating from its equilibrium position (indicated by the solid blue line) can be considered as a Brownian motion in the migration direction.**

to physically relevant temperatures. Deng and Schuh [26,27] proposed a novel postprocessing approach, which effectively increased the accuracy and extended the application of the interface random walk approach to low temperatures, up to 0.2 homologous temperature. Mobilities determined from the interface random walk have been shown to be consistent with those obtained from other molecular dynamics simulation approaches based on driving forces [28,29]. Over the past decade, the interface random walk method has been successfully applied to estimate the mobility of impurity-free grain boundaries [16,26,27] and boundaries with impurity atoms [30,31].

## 4 Impact of Defects on Interfacial Fluctuations

The approaches outlined above have mostly been used to elucidate the properties of pristine interfaces. However, they also open fascinating avenues to study interactions between defects or defective interfaces. Here, we present two example cases where mechanistic insights can be gleaned from how interfacial fluctuations are impacted by the presence of defects.

**4.1 Effect of Entropic Interactions Between Fluctuating Interfaces.** The idea that a fluid membrane fluctuating close to adjacent surfaces, such as in a multilayer system, experiences an effective repulsive entropic pressure was first introduced in the pioneering work of Helfrich [5]. Since then, it has been revisited theoretically and via atomistic simulations in recent years [6,7]. Unlike an unconfined or free membrane, when membranes are fluctuating close to each other, there is a constraint on the out-of-plane deflection ($h(x)$) due to confinement, such that $-d \leq h(x) \leq d$, where the membranes are separated by a distance $2d$. A "soft constraint" is often used to replace the inequality, in which the membrane is subjected to an effective harmonic (constraining) potential [32]. Applying this idea to the case of crystalline interfaces that exhibit capillary fluctuations, the energy in Eq. (2) becomes

$$E = \frac{1}{2} b \int_0^W \left[\Gamma h_x^2 + \eta h^2(x)\right] dx \tag{9}$$

where $\eta$ is a positive constant, and the new energy term accounts for the confinement. Following the procedure outlined before, the modified fluctuation spectrum is obtained as

$$\langle |A(k)|^2 \rangle = \frac{k_B T}{bW(\Gamma k^2 + \eta)} \tag{10}$$

The equation reveals that the effect of $\eta$ can be ignored for small wavelength. However, at long wavelength or small $k$, $\eta$ is the dominant term, and the fluctuation spectrum essentially becomes independent of $k$. This implies that the steric interaction between interfaces is repulsive in nature and inhibits their fluctuations especially in the long wavelength modes. The repulsive nature of the entropic force and the concomitant suppression of fluctuations have also been reported in the study of entropic interactions between solid–liquid interfaces [15] and crystalline membranes such as bilayer graphene [33] using atomistic simulations.

On a rather intriguing note, crystalline interfaces that have a propensity for shear-coupled normal motion exhibit a dramatically opposite behavior. Recent molecular dynamics simulations by Chen and Kulkarni [34] revealed that the interaction between parallel coherent twin boundaries results in enhanced thermal fluctuations. It is further corroborated by their theoretical analysis which shows that fluctuating twin boundaries indeed exhibit an attractive entropic interaction, enhancing their fluctuations. This is attributed to the characteristic of these twin boundaries to exhibit shear-coupled normal motion. Figure 7 compares the molecular dynamics simulation results for a high-angle $\Sigma5(210)$ grain boundary and $\Sigma3(111)$ coherent twin boundary which show opposite behavior of the long wavelength modes due to entropic interactions. Interestingly, Rickman and Lesar [35] also found an attractive force between dislocation lines when entropic effects are taken into account.

**4.2 Effect of Impurities on Interface Mobility.** Impurities, such as second-phase particles, defect clusters, or interstitial solute atoms, are known to dramatically influence grain boundary migration, thereby impacting material properties. Following the linear relation in Eq. (6), the influence of the impurities is captured by their impact on the mobility, often reducing it by orders of magnitude [36]. In fact, it is generally accepted that the large discrepancies found between mobilities predicted by modeling (of perfect interfaces) and those estimated from experiments are due to the drag effect of impurities invariably present in experimental specimens.

Thermal fluctuations, and specifically, the interface random walk approach, offer a unique way to quantify the drag effect of impurities on grain boundary mobility, which has been difficult to ascertain experimentally due to the lack of controlled experiments on individual grain boundaries. Recent computational studies, based on the interface random walk approach, by Sun and Deng

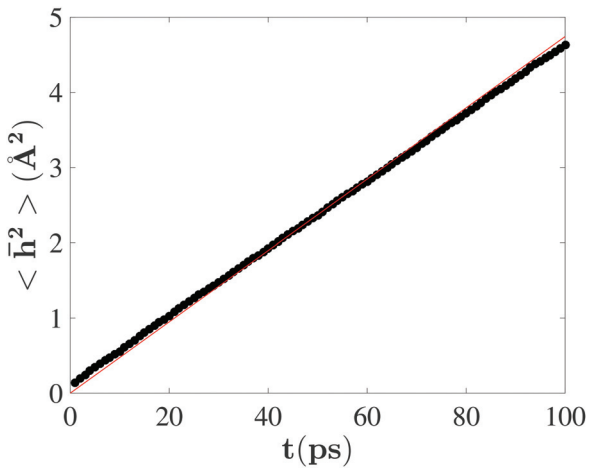


**Fig. 5 Temporal evolution of the variance $\langle \bar{h}^2 \rangle$ for the $\Sigma17(410)$ grain boundary in Ni at 1200 K. The dots represent simulation data, while the solid red line shows the linear fit of the form $\langle \bar{h}^2 \rangle = Dt$. Computing $D$ from this plot yields the mobility. The simulations were performed in LAMMPS [17] using the EAM interatomic potential developed by Baskes and co-workers [24,25].**

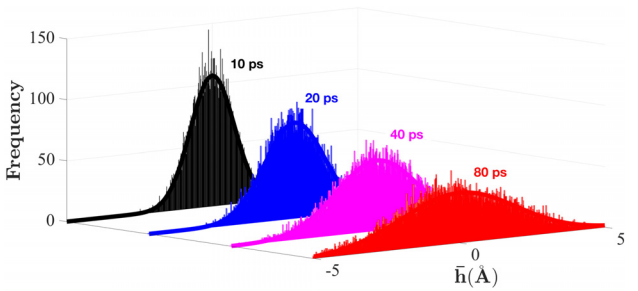


**Fig. 6 Distribution of the average interface position $\bar{h}(t)$ with respect to the initial position ($\bar{h}(0) = 0$) at different time intervals obtained from molecular dynamics. The results are for the case of a $\Sigma17(410)$ grain boundary in Ni at 1200 K. The Gaussian form $f = Be^{-\alpha \bar{h}^2}$ is fitted to the data and shown by solid lines, where $B$ and $\alpha$ are measures of the height and width of the distribution, respectively. The simulations were performed in LAMMPS [17] using the EAM interatomic potential developed by Baskes and co-workers [24,25].**

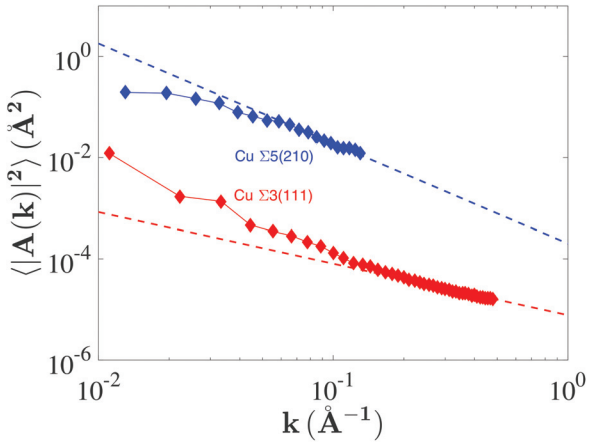


**Fig. 7 Fluctuation spectra as a function of wave number *k* for Σ3(111) twin boundary (in red) and Σ5(210) high-angle grain boundary (in blue) obtained from molecular dynamics. The high angle grain boundary shows suppressed fluctuations due to neighboring grain boundaries thus deviating from the linear dependence with −2 slope (shown by blue dashed line) at long wavelengths. In contrast, the twin boundary shows enhanced fluctuations due to neighboring twin boundaries thus deviating from the linear dependence with −1 slope (shown by red dashed line) at long wavelengths. The simulations were performed in LAMMPS [17] using the EAM interatomic potential for Cu developed by Mishin et al. [18].**

[30,31] show that the mobility of grain boundaries decreases by an order of magnitude with increasing density of solute atoms segregated at the interface. In fact, the mobility obtained from atomistic simulations is found to be consistent with the solute drag model proposed by Cahn [37] and Lücke and Stüwe [38] (referred to as the CLS model) thereby validating its predictions. Thus, thermal fluctuations-based methods proffer a unique capability to combine analytical models such as the CLS model for solute drag effect or the Zener model for particle pinning [39,40] developed almost five decades ago, with large-scale atomistic simulation methods to perform quantitative studies on the effect of impurities on grain boundary migration.

## 5 Future Directions

In this perspective article, we put forward our viewpoint that thermal fluctuations of crystalline interfaces, despite being on the scale of a few nanometers, can serve as a computational microscope for gaining insights into equilibrium and nonequilibrium properties of grain boundaries. To this end, we reviewed some major developments in the area, specifically, the application of membrane theory to obtain important interfacial parameters such as grain boundary free energy and stiffness, and the treatment of fluctuating interfaces as Brownian particles to compute their mobilities.

These approaches suggest exciting routes for probing a variety of open questions germane to interfaces and critical phenomena where interfaces are known to be key players such as creep, grain growth, dendritic solidification among others. What is the nature of the interaction between grain boundaries and other defects such as dislocations or stacking faults? Addressing this question would entail the study of the thermal fluctuations of different line and planar defects. Another compelling avenue is the study of the sliding mobilities of grain boundaries via thermal fluctuations to establish the structure and temperature dependence of grain boundary sliding, a critical player in creep of polycrystalline materials. The interface random walk method provides a fresh path for probing the pinning effect of second-phase particles on interfacial migration and furnishing atomistic evidence into a process that has largely been studied via analytical models. We believe that it would be quite revealing to explore phenomena such as void formation and growth, and edge effects in crystalline boundaries from the standpoint of thermal fluctuations. This could provide new atomistic insights into void nucleation, a major phenomenon in high temperature damage in materials. Physical quantities associated with individual interfaces extracted from equilibrium fluctuations can also serve as input for coarse-grained computational models to predict the overall mechanical response of polycrystalline materials. A very appealing but yet uncharted territory is to extend these thermal fluctuations based methods to examine interfacial properties that play a role in electromechanical-coupled phenomena which could have wide technological applications. These fascinating avenues support our argument that the statistical mechanics of crystalline interfaces indeed presents a rich source for future study.


## Acknowledgment

The authors also acknowledge the use of the Maxwell cluster and the support from the Center of Advanced Computing and Data Systems at the University of Houston to carry out the research presented here.

## Funding Data

- Directorate for Engineering (Grant No. CMMI-1129041).
- Directorate for Mathematical & Physical Sciences (Grant No. DMR-1508484).


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