Coarse-Graining and Renormalization of Atomistic Binding Relations and Universal Macroscopic Cohesive Behavior

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Abstract

We present two approaches for coarse-graining interplanar potentials and determining the corresponding macroscopic cohesive laws based on energy relaxation and the renormalization group. We analyze the cohesive behavior of a large—but finite—number of interatomic planes and find that the macroscopic cohesive law adopts a universal asymptotic form. The universal form of the macroscopic cohesive law is an attractive fixed point of a suitably-defined renormalization-group transformation.

1 Introduction

Cohesive theories of fracture are predicated on a direct description of the physical processes which lead to separation and the eventual formation of a free surface. The development of cohesive theories rests on a detailed physical understanding of the operative fracture mechanisms, which are often complex and cut across multiple lengthscales, especially where ductile fracture is concerned. Cleavage fracture, by way of contrast, entails the simple separation of atomic planes and is, therefore, governed by interplanar potentials which are amenable to an effective first-principles atomistic characterization. For instance, Jarvis et al. [6] have recently calculated the cohesive behavior of (111) planes in fcc aluminum, and of Al$_2$O$_3$ cleavage planes, using GGA density functional theory; and Park and Kaxiras [7] have carried out ab-initio simulations of hydrogen embrittlement in aluminum and calculated generalized stacking-fault energies as a function of interplanar separation and sliding.

First-principles interplanar potentials are characterized by peak stresses of the order of the theoretical strength of the crystal. In addition, the crystal loses its bearing capacity after an interplanar separation of only a few angstroms.
Moreover, the integration of first-principles interplanar potentials into engineering calculations necessitates full atomistic resolution in the vicinity of the crack tip, which is often unfeasible or impractical. This disconnect between atomistic and engineering descriptions begs a number of fundamental questions, to wit: What is the proper way to coarse-grain a cohesive description?, and: What is the macroscopic form of the cohesive law after coarse-graining?

In this paper we address these issues by investigating the cooperative behavior of a large number of interatomic planes forming a cohesive layer. We employ two main approaches in this investigation: relaxation and the renormalization group. Relaxation or weak convergence methods are concerned with the determination of the macroscopic behavior of materials characterized by a non-convex energy function. These materials often develop fine microstructure in response to imposed deformations. Truskinovsky et al. [3, 8, 4], and Braides et al. [2], have pioneered the application of these methods to fracture. However, the full relaxation of a cohesive potential yields the trivial result that the effective cohesive potential is identically equal to zero. The chief difference between the analysis pursued here and full relaxation is that, at zero temperature, we seek energy minimizers of large— but finite—collections of interatomic planes. In this limit we find that, for a broad class of interpl anar potentials, the macroscopic cohesive law adopts a universal form asymptotically.

We show that this universality of the macroscopic cohesive behavior is amenable to a renormalization-group interpretation. The normalization group which coarse-grains the cohesive behavior is somewhat nonstandard and has to be crafted carefully, e. g., so as to preserve the surface energy and the elasticity of the lattice. The universal form of the macroscopic cohesive law is precisely an attractive fixed point of the renormalization-group transformation.

2 Problem formulation

We consider a macroscopic cohesive crack opening symmetrically (mode I) and undergoing quasistatic growth. We denote by $d$ the interplanar distance, $\delta$ the opening displacement across an interatomic plane, and $t$ the corresponding cohesive traction. These latter variables are presumed related by a known cohesive or binding law $t(\delta)$, which derives from an interplanar potential $\phi(\delta)$ through the relation:

$$t(\delta) = \phi'(\delta)$$

Here and subsequently, a prime denotes differentiation of a function of a single variable. For simplicity, we shall assume throughout that the atomistic binding law $t(\delta)$ rises monotonically from zero at $\delta = 0$ to a peak value $\sigma_c$ at $\delta = \delta_c$, and subsequently decreases monotonically to zero, Fig. 1. Correspondingly, the cohesive potential $\phi(\delta)$ is convex in the interval $0 \leq \delta < \delta_c$, is concave for $\delta > \delta_c$ and asymptotes to twice the surface energy, $2\gamma$, as $\delta \to \infty$. In addition, we shall assume that $\phi(\delta)$ is smooth and analytic at $\delta = 0$, with Taylor expansion:

$$\phi \sim \frac{C}{2} \delta^2 + o(\delta^2)$$
for some constant $C$. The value of $C$ can be readily deduced from the elastic moduli $c_{ijkl}$ of the crystal. To this end, let $\mathbf{m}$ be the unit normal to the plane of the crack, and apply a small and uniform opening displacement to all interatomic planes. Evidently, the energy per unit volume of the crystal follows from the cohesive potential as $(C/2d)\delta^2$ asymptotically as $\delta \to 0$. On the other hand, the strain tensor of the crystal is $\epsilon_{ij} = (\delta/d)m_im_j$, and the corresponding energy is $(\delta^2/2d^2)c_{ijkl}m_im_jm_km_l$. Equating both energies yields the identity:

$$C = \frac{1}{d}c_{ijkl}m_im_jm_km_l$$

Next imagine that the atomistic description is coarse-grained, e. g., by the quasi-continuum method [10], or by a passage to the continuum limit, or by some other suitable means. Let $\tilde{d}$ denote the spatial resolution of the coarse-grained description. For instance, in quasicontinuum or in engineering finite-element simulations $\tilde{d}$ measures the local element size. The corresponding effective cohesive law may be obtained by analyzing the behavior of a cohesive layer of thickness $\tilde{d}$ and containing $N = \tilde{d}/d$ atomic planes. The cohesive layer is taken through a total opening displacement $\tilde{\delta}$ resulting in a macroscopic traction $\tilde{t}$. The chief objective of the analyses that follow is to determine the macroscopic cohesive law $\tilde{t}(\tilde{\delta})$ in the limit of $N$ large but finite. Equivalently, we may seek to determine the asymptotic form of the macroscopic cohesive

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Figure 1: Interplanar potential and corresponding cohesive or binding law.
potential $\bar{\phi}(\bar{\delta})$ such that

$$\bar{t}(\bar{\delta}) = \bar{\phi}'(\bar{\delta})$$

in the same limit.

### 3 Universal asymptotic form of the macroscopic cohesive law at zero temperature

At zero temperature, the crystal deforms so as to minimize its total energy. The governing principle is, therefore, energy minimization. Let $\delta_i \geq 0, i = 1, \ldots, N$ be the opening displacements of the interatomic planes in the cohesive layer. Then, the total energy of the cohesive layer is:

$$E^{\text{tot}} = \sum_{i=1}^{N} \phi(\delta_i)$$

Let now $\bar{\delta}$ be the macroscopic opening displacement. Then, the effective or macroscopic energy of the cohesive layer follows from the constrained minimization problem:

$$\bar{\phi}(\bar{\delta}) = \inf_{\{\delta_1, \ldots, \delta_N\}} \sum_{i=1}^{N} \phi(\delta_i)$$

$$\bar{\delta} = \sum_{i=1}^{N} \delta_i$$

In conjunction with the kinematic constraints, the stationarity of $E^{\text{tot}}$ demands:

$$t(\delta_i) = \bar{t}(\bar{\delta}) = \text{constant}, \quad i = 1, \ldots, N$$

Thus, at equilibrium, all interplanar tractions must be equal to the macroscopic traction.

We shall classify the possible states of an interatomic plane into two categories or variants, according as to whether the opening displacement $\delta$ is in the range $0 \leq \delta < \delta_c$, or in the range $\delta > \delta_c$. We shall designate variants of the first kind as coherent, and variants of the second kind as decohered. We may further classify the states of a cohesive layer by the number $N_1$ of coherent planes, or, equivalently, the number $N_2$ of decohered planes, it contains. Since the function $t(\delta)$ is one-to-one over the interval $[0, \delta_c)$, eq. (8) demands that the opening displacements of all coherent planes be equal at equilibrium. Likewise, the opening displacements of all decohered planes must be identical at equilibrium. Under these conditions the macroscopic cohesive energy follows
from the minimization problem:

\[
\bar{\phi}(\bar{\delta}) = \inf_{\{N_1, N_2\}, (\delta_1, \delta_2)} \{N_1 \phi(\delta_1) + N_2 \phi(\delta_2)\} \quad (9)
\]

\[
\bar{\delta} = N_1 \delta_1 + N_2 \delta_2 \quad (10)
\]

\[
N = N_1 + N_2 \quad (11)
\]

\[
0 \leq \delta_1 < \delta_c \quad (12)
\]

\[
\delta_2 > \delta_c \quad (13)
\]

where \(\delta_1\) and \(\delta_2\) are the opening displacements in the coherent and decohered planes, respectively. In addition, the equilibrium equations (8) reduce to:

\[
t(\delta_1) = t(\delta_2) = \bar{t}(\bar{\delta}) \quad (14)
\]

These relations are depicted geometrically in Fig. 1.

Next we proceed to determine the minimum energy states of a cohesive layer by analyzing the cases \(N_2 = 0, 1, 2, \ldots\) in turn. We begin by considering the case in which all planes are coherent, corresponding to \(N_1 = N\) and \(N_2 = 0\). Then, the kinematic constraint (10) gives \(\delta_1 = \bar{\delta}/N \equiv \delta\). Evidently, in the limit of \(N \to \infty\) \(\delta\) tends to zero and, in view of eqs. (2) and (9), we obtain:

\[
\bar{\phi}(\delta) \big|_{N_2=0} \sim \frac{C}{2} \delta^2, \quad \text{as } N \to \infty \quad (15)
\]

where

\[
\bar{C} = \frac{C}{N} \quad (16)
\]

is an effective cohesive-layer stiffness.

Consider next the case of one decohered plane, \(N_1 = N - 1\) and \(N_2 = 1\), whence (14) becomes:

\[
(N - 1) \delta_1 + \delta_2 = \bar{\delta} \quad (17)
\]

Solving for \(\delta_1\) gives \(\delta_1 = (\bar{\delta} - \delta_2)/(N - 1)\). In addition, since \(\delta_i\) and \(\bar{\delta}\) are required to be nonnegative, it follows that \(\delta_1 \leq \bar{\delta}/(N - 1)\), and thus \(\delta_1 \to 0\) as \(N \to \infty\). From this limit it additionally follows that \(\delta_2 \to \bar{\delta}\) in the same limit. Suppose now that \(\bar{\delta} \gg \delta_c\) and, hence, \(\delta_2 \gg \delta_c\). Under these conditions, \(\phi(\delta_2) \sim 2\gamma\) and (14) reduces to:

\[
\bar{\phi}(\bar{\delta}) \big|_{N_2=1} \sim 2\gamma, \quad \text{as } N \to \infty \quad (18)
\]

Since interactions beyond nearest neighbors are not taken into account, an altogether identical analysis gives

\[
\bar{\phi}(\delta) \big|_{N_2=k} \sim 2k\gamma, \quad \text{as } N \to \infty \quad (19)
\]

for the case of \(k\) decohered planes.

The macroscopic cohesive energy may now be expressed as

\[
\bar{\phi}(\delta) = \min_{0 \leq k \leq N} \bar{\phi}(\delta) \big|_{N_2=k} \quad (20)
\]
However, it follows from (19) that, asymptotically as $N \to \infty$, multiple decohered planes are not energetically possible at zero temperature, and only the cases $k = 0$ and $k = 1$ need be considered in (20). Therefore, the effective cohesive potential is the lower envelop of the energies (15) and (18), namely,

$$\bar{\phi}(\bar{\delta}) = \min\{\frac{\bar{C}}{2}\bar{\delta}^2, 2\gamma\} = \begin{cases} \frac{(\bar{C}/2)\bar{\delta}^2}{2\gamma}, & \text{if } \bar{\delta} < \bar{\delta}_c \\ 2\gamma, & \text{otherwise} \end{cases}$$

(21)

where

$$\bar{\delta}_c = 2\sqrt{\gamma} = 2\sqrt{\gamma N / C}$$

(22)

is a macroscopic critical opening displacement for the nucleation of a single decohered plane. The corresponding macroscopic cohesive law is

$$\bar{t}(\bar{\delta}) = \begin{cases} \bar{C}\bar{\delta}, & \text{if } \bar{\delta} < \bar{\delta}_c \\ 0, & \text{otherwise} \end{cases}$$

(23)

It is interesting to note that the peak macroscopic traction is:

$$\bar{\sigma}_c = \bar{C}\bar{\delta}_c = 2\sqrt{\gamma} = 2\sqrt{\gamma N / C}$$

(24)

We conclude the analysis by verifying that, in the decohered regime, $\bar{\delta} > \bar{\delta}_c \sim \sqrt{N}$, and hence $\bar{\delta} \gg \delta_c$ for sufficiently large $N$, as supposed.

These functions are shown in Fig. 2. The macroscopic cohesive potential is initially quadratic and subsequently constant following the attainment of the critical macroscopic opening displacement. Remarkably, the macroscopic critical opening displacement and peak traction scale as: $\bar{\delta}_c \sim \sqrt{N}$ and $\bar{\sigma}_c \sim 1/\sqrt{N}$, respectively. Thus, for large $N$, it follows that the macroscopic cohesive law entails much lower tractions, occurring at much larger opening displacements, than the atomistic binding law. In effect, the passage from the atomistic to the macroscopic scales is accompanied by an expansion of the opening displacement axis and a simultaneous compression of the traction axis. By contrast, the macroscopic fracture energy, or critical energy-release rate, $\bar{\phi}(\infty)$ remains invariant under the transformation and is equal to the atomistic value $\phi(\infty) = 2\gamma$. It is also remarkable that, for the class of binding laws under consideration, the asymptotic form (21) of the macroscopic cohesive law is universal, i.e., independent of the atomistic binding law. Evidently, the parameters which define the macroscopic cohesive law quantitatively, e.g., the surface energy $\gamma$ and the modulus $C$, are material specific.

As a simple illustrative example we consider the universal binding energy relation (UBER) defined by the interplanar potential:

$$\phi(\delta) = 2\gamma - C\delta_0(\delta + \delta_c)e^{-\delta/\delta_c}$$

(25)

This function falls within the class of potentials considered in the foregoing. We choose as material constants: $C = 3.54 \text{ J/m}^2/\text{Å}^2$, $\delta_c = 0.66 \text{ Å}$, which are representative of aluminum. The macroscopic cohesive laws resulting from a direct numerical minimization of the energy (21) for different values of $N$ are
shown in Fig. 3. The universal asymptotic form of the macroscopic cohesive law is compared in Fig. 4 against the corresponding numerical results. The convergence of the macroscopic cohesive law towards the universal asymptotic form as the number of planes in the cohesive layer increases is clearly evident in this figure.

4 Effect of finite temperature

At finite temperature, entropic effects make it feasible for the cohesive layer to decohere on multiple planes. In order to assess this effect simply, we recall that, asymptotically, the energy of a cohesive layer with no decohered planes is \((C/2)\delta^2\), and that the energy of a cohesive layer containing \(k\) decohered planes is \(2k\gamma\). Within this approximation, the partition function of an area \(a^2\) of layer is, therefore,

\[
Z(\bar{\delta}, T) = e^{-\bar{\beta}(C/2)\bar{\delta}^2} a^2 + \sum_{k=1}^{\infty} e^{-\bar{\beta}2k\gamma a^2}
\]  

(26)

where \(\bar{\beta} = 1/kT\), and \(k\) is Boltzmann’s constant. In order to count states properly, we identify \(a\) with the lattice parameter of the crystal. Physically, this is tantamount to allowing for decohered areas of a size commensurate with

Figure 2: Universal asymptotic form of the macroscopic cohesive law at zero temperature.
Figure 3: Numerically computed macroscopic traction vs opening displacement relation for an increasing number of atomic planes in the cohesive layer.

The lattice parameter. The sum in (26) defines a geometric series which may be evaluated readily, with the result:

\[ Z(\tilde{\delta}, T) = e^{-\beta(\bar{C}/2)\tilde{\delta}^2a^2} + \frac{e^{-\bar{\gamma}a^2}}{1 - e^{-\bar{2}\gamma a^2}} \]  

(27)

The free energy density per unit area of the layer now follows as

\[ \bar{F}(\tilde{\delta}, T) = -\frac{1}{a^2 \beta} \log Z(\tilde{\delta}, T) \]  

(28)

whereas the resulting effective cohesive law is:

\[ \bar{t}(\tilde{\delta}, T) = \frac{d\bar{F}}{d\tilde{\delta}}(\tilde{\delta}, T) \]  

(29)

The effect of temperature on the macroscopic cohesive potential for aluminum, endowed with an interplanar potential of the UBER type, is shown in Fig. 5a. The lattice parameter is taken to be \( a = 4.05 \) Å. As expected, the Helmholtz free energy rises above the zero-temperature in the amount \( TS \), where \( S \) is the configurational entropy of the layer, Fig. 5a. The corresponding effect on the macroscopic cohesive law is to smooth out the decohesion transition, Fig. 5b.

5 Renormalization Group interpretation

The renormalization group (RG) (see, e.g., [4]) provides a natural framework for the understanding of universality, i.e., the phenomenon that large classes of
Figure 4: Comparison between numerically computed macroscopic cohesive law and universal asymptotic form for an increasing number of atomic planes in the cohesive layer.
systems with unrelated Hamiltonians may nevertheless exhibit identical thermodynamic behavior near critical points. It is therefore not entirely unexpected that the main result of Section 3, namely, that the limiting form of the potential of a cohesive layer is universal for a broad class of interplanar potentials, can be given a compelling interpretation within the RG framework.

For simplicity, we confine our attention to the zero temperature case. We proceed to construct an RG transformation $R$ such that the sequence

$$\phi_{n+1} = R\phi_n, \quad n = 0, 1, \ldots$$

(30)

with $\phi_0(\delta) = \phi(\delta)$, yields, by recourse to an appropriate scaling, the large $N$ asymptotic form of the macroscopic cohesive law in the limit. As in the preceding section, the interplanar potentials contemplated here, and to which the transformation $R$ is applied, are continuous, monotonically increasing functions $\phi : [0, \infty) \rightarrow [0, 2\gamma]$ and analytic at the origin. For simplicity, we additionally restrict attention to functions $\phi(\delta)$ possessing a single inflection point, so that $\phi'(\delta)$ has a single maximum.

We construct $R$ by the usual combination of decimation and scaling. The decimation step concerns a layer consisting of two interatomic planes with opening displacements $\delta_1$ and $\delta_2$ and total opening displacement $\delta$. The corresponding effective energy follows from the minimization problem:

$$\tilde{\phi}(\delta) = \inf_{\{\delta_1, \delta_2\}} \{\phi(\delta_1) + \phi(\delta_2)\}$$

(31)

$$\delta = \delta_1 + \delta_2$$

(32)

Next, we proceed to rescale $\tilde{\phi}(\delta)$ in such a way that the sequence defined by (30) has a well-defined fixed point. Since the transformation must preserve the relation $\phi(\infty) = 2\gamma$, it is clear that we are allowed to rescale the independent variable $\delta$ only. Thus, we set:

$$(R\phi)(\delta) = \tilde{\phi}(\lambda\delta)$$

(33)

For very small $\delta$ the interplanar potential $\phi$ is essentially quadratic and reflects the elasticity of the lattice. Thus, in order for the transformation to preserve the elasticity of the lattice it must leave parabolic functions invariant. For $\phi = (C/2)\delta^2$ it follows that $\delta_1 = \delta_2 = \delta/2$ and $\tilde{\phi} = 2(C/2)(\delta/2)^2 = (C/2)(\delta/\sqrt{2})^2$. Finally, $(R\phi)(\delta) = (C/2)(\lambda\delta/\sqrt{2})^2$, whence it follows that $\lambda = \sqrt{2}$ for $\phi$ to remain invariant under the transformation. The complete RG transformation is, therefore,

$$\tilde{\phi}(\delta) = \inf_{\{\delta_1, \delta_2\}} \{\phi(\delta_1) + \phi(\delta_2)\}$$

(34)

$$\delta = \delta_1 + \delta_2$$

(35)

$$(R\phi)(\delta) = \tilde{\phi}(\sqrt{2}\delta)$$

(36)

Taking $\delta_1 = 0$ and $\delta_2 = \delta$ in (34) immediately shows that the unscaled energy $\tilde{\phi}(\delta)$ is bounded above by the original function $\phi(\delta)$.

It is clear from definition (34-36) that the RG transformation leaves the specific fracture energy $\phi(\infty)$ invariant and equal to its initial value $2\gamma$. Another
invariant of the RG transformation is the initial modulus $C = \phi^\circ(0)$. Indeed, consider the limit of $R\phi$ as $\delta \to 0$. Since necessarily $\delta_1 < \delta$ and $\delta_2 < \delta$ it follows that both $\delta_1 \to 0$ and $\delta_2 \to 0$ in this limit. $(R\phi)(\delta)$ may therefore be computed by replacing $\phi(\delta)$ by its Taylor expansion about the origin, namely, $(C/2)\delta^2$, with $C = \phi^\circ(0)$. But parabolic functions are invariant under $R$ and, hence, so is $C$.

The RG transformation $R$ preserves the monotonicity of $\phi(\delta)$. In order to see this, consider a pair of opening displacements $\delta$ and $\lambda < 1$. Let $\tilde{C} = C$ in order to see this, consider a pair of opening displacements $\phi$ by replacing $\delta$ order to see this, consider a pair of opening displacements $\phi$ by replacing $\delta$ and $\lambda \delta < 1$ with $\phi$ that both $\tilde{C}$ is invariant of the RG transformation is the initial modulus $C = \phi^\circ(0)$. Indeed, consider the limit of $R\phi$ as $\delta \to 0$. Since necessarily $\delta_1 < \delta$ and $\delta_2 < \delta$ it follows that both $\delta_1 \to 0$ and $\delta_2 \to 0$ in this limit. $(R\phi)(\delta)$ may therefore be computed by replacing $\phi(\delta)$ by its Taylor expansion about the origin, namely, $(C/2)\delta^2$, with $C = \phi^\circ(0)$. But parabolic functions are invariant under $R$ and, hence, so is $C$.

The RG transformation $R$ preserves the monotonicity of $\phi(\delta)$. In order to see this, consider a pair of opening displacements $\delta$ and $\delta' = \lambda \delta$, with $\lambda < 1$. Let $\tilde{\phi}(\delta) = \phi(\delta_1) + \phi(\delta_2)$ for some pair of opening displacements $\delta_1$ and $\delta_2$ satisfying constraint \((35)\). The opening displacements $\delta'_1 = \lambda \delta_1$ and $\delta'_2 = \lambda \delta_2$ then satisfy the similar constraint: $\delta' = \delta'_1 + \delta'_2$. It therefore follows that $\tilde{\phi}(\delta') < \phi(\lambda \delta_1) + \phi(\lambda \delta_2) < \phi(\delta_1) + \phi(\delta_2) = \tilde{\phi}(\delta)$. An application of the rescaling \((36)\) to both sides of this inequality finally proves the assertion.

It is easy to show that the function:

$$\phi_{\infty}(\delta) = \min\{C, 2\delta^2\}$$

is a fixed point of $R$. To this end, we may distinguish the cases: a) $\delta_1 < \delta_2$ and $\delta_2 < \delta_\circ$; b) $\delta_1 < \delta_\circ$ and $\delta_2 > \delta_\circ$, or, equivalently, $\delta_2 < \delta_\circ$ and $\delta_1 > \delta_\circ$, and c) $\delta_1 > \delta_2$ and $\delta_2 > \delta_\circ$. Case (a) requires that $\delta < 2\delta_\circ$ and gives an unscaled energy: $\tilde{\phi}(\delta) = (C/2)(\delta/\sqrt{2})^2$. Case (b) requires that $\delta > \delta_\circ$. The optimal unscaled energy is obtained by taking $\delta_1 = 0$ and $\delta_2 = \delta$, with the result: $\tilde{\phi}(\delta) = 2\gamma$. Case (c) results in the unscaled energy: $\tilde{\phi}(\delta) = 4\gamma$. The function \((37)\) is recovered by taking the minimum of the unscaled energies resulting from cases (a), (b) and (c) and applying the scaling \((36)\) to the result.

A key question is whether the fixed point \((37)\) is attractive. We have investigated this question numerically for the particular example of the UBER binding law \((23)\). Fig. 1 shows the evolution of $\phi_n$ with increasing $n$. It is clear from the figure that, at least for the example under consideration, the flow of functions $\phi_n(\delta)$ does indeed converge strongly to the fixed point \((37)\). The relation to the asymptotic cohesive law \((21)\) is as follows. We may regard $\phi_n(\delta)$ as the result of decimating and rescaling $n$ times a cohesive layer containing $N = 2^n$ planes. The total opening displacement of the layer is obtained by undoing all the rescalings, with the result: $\tilde{\delta} = (\sqrt{2})^n \delta = \sqrt{N}\delta$. For large $N$, $\phi_n(\delta) \sim \phi_{\infty}(\delta)$ and one has

$$\phi(\delta) \sim \phi_{\infty}(\delta/\sqrt{N}), \quad \text{as } N \to \infty$$

which is identical to \((21)\).

Eq. \((38)\) establishes a connection between the renormalization group, specifically as generated by transformation \((34-36)\), and the large-$N$ asymptotic form of the cohesive potential determined directly in the preceding section. It is interesting to note that the RG transformations which pertain to the renormalization of interplanar potentials are markedly different from those which arise in the calculation of bulk thermodynamic properties. In this latter context, the appropriate scaling is related to the volume of the sample and is designed so as to result in well-defined extensive fields and intensive variables. In the present context, the energy densities under consideration are defined per unit area, and
the limit of interest is the total energy of the cohesive layer per unit surface area, as opposed to the energy per unit volume. In addition, the independent variable of interest is the total opening displacement across the cohesive layer, as opposed to its transverse strain. These peculiarities account for the non-standard character of the renormalization group defined in the foregoing.

6 Summary and conclusions

We have presented two approaches for coarse-graining interplanar potentials and determining the corresponding macroscopic cohesive laws based on energy relaxation and the renormalization group. We have analyzed the cohesive behavior of a large—but finite—number $N$ of interatomic planes and found that the macroscopic cohesive law adopts a universal asymptotic form in the limit of large $N$. We have also found that this asymptotic form of the macroscopic cohesive law is an attractive fixed point of a suitably-defined renormalization-group transformation.

The universal asymptotic form of cohesive law is particularly simple: the traction rises linearly from zero to a peak stress $\bar{\sigma}_c$ at a critical opening displacement $\bar{\delta}_c$, and subsequently drops to zero. The scaling of the peak stress and critical opening displacement is $\bar{\delta}_c \sim 1/\sqrt{N}$ and $\bar{\sigma}_c \sim \sqrt{N}$. Thus, coarse-graining is accompanied by an attendant reduction (increase) in the cohesive traction (opening displacement) range, while at the same time preserving the surface of specific fracture energy of the crystal.

It is interesting to note that the size of a cohesive zone at the tip of a crack in an elastic crystal scales as $l \sim 1/\sigma_c^2$. Upon coarse-graining, the cohesive zone size increases to $\bar{l} \sim 1/\bar{\sigma}_c^2$, which gives $\bar{l} \sim Nl$. This scaling preserves the ratio $\bar{l}/l = d/d$, which shows that coarse-graining has the effect of expanding the cohesive-zone size to within the resolution of the coarse-grained description. In particular, it eliminates the onerous need to resolve the atomic scale in simulations.

It is also interesting to note that the universal form of the macroscopic cohesive potential is completely determined by the constants $C = \phi''(0)$ and $\phi(\infty) = 2\gamma$. This greatly reduces the scope of the first-principles calculations required to identify the macroscopic cohesive behavior of specific materials, which can be limited to the calculation of elastic moduli, lattice constants and surface energies.

Finally, we close by suggesting possible extensions of the theory. The analysis presented in the foregoing has been restricted to symmetric (mode I) opening normal to the atomic planes. A worthwhile extension would be to consider interplanar potentials defined in terms of three opening displacements and, therefore, capable of describing tension-shear coupling. Another worthwhile extension would be to consider interplanar potentials with multiple inflection points, which would greatly enlarge the class of materials tractable within the theory.
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Figure 5: Influence of the temperature on the effective behavior of the chain ($N = 100$).

(a) Helmholtz free energy.

(b) Macroscopic cohesive traction.
Figure 6: Evolution of the sequence $\phi_n$, $n = 0, 1, \ldots$ towards the fixed point $\phi_\infty$. 