Configurational Forces in Bond Order Potentials

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In this contribution, a configurational mechanics framework is elaborated to assess the applicability of atomistic configurational forces in fracture of crystalline lattices. To this end, an analytical interatomic potential is reformulated in terms of the material positions occupied by the atoms participating in two- and three-body interactions. It is demonstrated that such a potential satisfies the requirements of invariances i.e., translational, rotational and parity. The focus of this work is developing the configurational setting for the bond order Tersoff potential. Two-dimensional pre-cracked mono-layer graphene modelled with the Tersoff potential is chosen to study the configurational force approach in determining energy release during crack propagation into the lattice.

1 Introduction

Configurational mechanics is classically concerned with defects such as cracks and dislocations, which are embedded in the material and might evolve in it. The second-order Eshelby tensor [1] is the key element of configurational mechanics and allows for example the representation of path-independent integrals, such as \(J, L\) and \(M\) integrals [2]. Configurational forces [3], representing the divergence of the Eshelby tensor, appear in the vicinity of defects within the material. The realm of configurational mechanics is extended to discrete systems in [4]. We studied the application of atomistic configurational mechanics to two-dimensional crystalline lattices, which led to the notion of a Configurational-Force-Criterion for atomistic fracture [5].

Here, we systematize the notion of atomistic configurational forces for two- and three-body interatomic interactions. Therein, we consider energetic changes associated with material variations. We define material variations as the changes in two-body length and three-body area in the material configuration. We exemplify the configurational formulations for the bond order Tersoff potential [6] to examine the applicability of the theoretical framework to a fracture mechanics problem in a mono-layer graphene.

We organize this contribution as follows: after the introduction, Section 2 encompasses the notation and elaborates on the kinematics of the problem. In Section 3, we introduce two- and three-body potentials. Thereafter, we derive the governing configurational equations leading to the introduction of atomistic configurational two- and three-body forces. Moreover, the notion of atom-wise configurational force is presented for the configurational energy density of the Tersoff potential. For the sake of demonstration, we provide insights into the detailed analysis of configurational forces in a mono-layer graphene. Finally, Section 4 concludes the paper.

2 Quasi-static Kinematics

In the following, we define spatial and material kinematic quantities which are frequently used throughout the manuscript. We consider the relative vector between a pair of atoms as spatial and material pair length vectors

\[
\mathbf{x}_{\alpha\beta} := \mathbf{x}_\beta - \mathbf{x}_\alpha \quad \text{and} \quad \mathbf{X}_{\alpha\beta} := \mathbf{X}_\beta - \mathbf{X}_\alpha,
\]

where the magnitude of these vectors are denoted as spatial and material pair length

\[
x_{\alpha\beta} := |\mathbf{x}_{\alpha\beta}| \quad \text{and} \quad X_{\alpha\beta} := |\mathbf{X}_{\alpha\beta}|.
\]

Next, we describe three-body interaction as the area formed by the atomistic triplet as spatial and material three-body areas,

\[
a_{\beta\alpha\gamma} := |\mathbf{x}_{\alpha\beta} \times \mathbf{x}_{\alpha\gamma}| \quad \text{and} \quad A_{\beta\alpha\gamma} := |\mathbf{X}_{\alpha\beta} \times \mathbf{X}_{\alpha\gamma}|,
\]

which is accompanied by the introduction of spatial and material vectorial area elements,

\[
a_{\beta\alpha\gamma} := \mathbf{x}_{\alpha\beta} \times \mathbf{x}_{\alpha\gamma} \quad \text{and} \quad A_{\beta\alpha\gamma} := \mathbf{X}_{\alpha\beta} \times \mathbf{X}_{\alpha\gamma}.
\]

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Considering this parameterization, we define quantities representing the interatomic map from the material to the spatial configuration. A potential needs to satisfy the requirement of translational, rotational and parity invariance \[7\], we will thus employ a parameterization in terms of pair and triplet stretches. The pair stretch is defined as

\[ \Lambda_{\alpha\beta} := \frac{X_{\alpha\beta}}{x_{\alpha\beta}}, \]  
(5)

and triplet stretch takes the form,

\[ P_{\beta\alpha\gamma} := \frac{A_{\beta\alpha\gamma}}{a_{\beta\alpha\gamma}}. \]  
(6)

Moreover, we define material normal vectors facilitating the description of force. For a two-body interaction, we introduce material pair directions

\[ N_{\alpha\beta} := \frac{X_{\alpha\beta}}{X_{\alpha\beta}}, \]  
(7)

similarly, for a three-body interaction we denote the material triplet normals describing the directional area elements as

\[ N_{\beta\alpha\gamma} := \frac{A_{\beta\alpha\gamma}}{A_{\beta\alpha\gamma}}. \]  
(8)

The cosine maps of atomistic triplet angle at spatial and material configurations, \( \theta_{\alpha\beta\gamma} \) and \( \Theta_{\alpha\beta\gamma} \), respectively, are approximated with third degree Maclaurin polynomial function. That is,

\[ \cos \theta_{\beta\alpha\gamma} \approx 1 - \frac{\theta^2_{\beta\alpha\gamma}}{2} \quad \text{and} \quad \cos \Theta_{\beta\alpha\gamma} \approx 1 - \frac{\Theta^2_{\beta\alpha\gamma}}{2}, \]  
(9)

similarly, a second degree Maclaurin polynomial function is used to express \( \sin \theta_{\beta\alpha\gamma} \) and \( \sin \Theta_{\beta\alpha\gamma} \),

\[ \sin \theta_{\beta\alpha\gamma} \approx \theta_{\beta\alpha\gamma} \quad \text{and} \quad \sin \Theta_{\beta\alpha\gamma} \approx \Theta_{\beta\alpha\gamma}. \]  
(10)

Therefore, we can define the area of a triangle formed by the atomistic triplet in the spatial and material configurations as

\[ a_{\beta\alpha\gamma} = \frac{1}{2} x_{\alpha\beta} x_{\alpha\gamma} \theta_{\beta\alpha\gamma}. \quad \text{and} \quad A_{\beta\alpha\gamma} = \frac{1}{2} X_{\alpha\beta} X_{\alpha\gamma} \Theta_{\beta\alpha\gamma}. \]  
(11)

When taking into account the configurational triplet twist as,

\[ \Omega_{\beta\alpha\gamma} = \frac{\Theta_{\beta\alpha\gamma}}{\theta_{\beta\alpha\gamma}}. \]  
(12)

We can finally define the material triplet stretch using the pair stretch and triplet twist, such that,

\[ P_{\alpha\beta\gamma} = \Lambda_{\alpha\beta} \Lambda_{\alpha\gamma} \Omega_{\beta\alpha\gamma}. \]  
(13)

The applicability of the proposed kinematical quantities in the description of the potential energy density will be presented in the following sections.

![Fig. 1: Atomistic motion from material position to spatial position. The area and directional area formed by a triplet of atoms as well as interatomic pair vectors are illustrated.](H:\PROJ\AA\2021-08-25_Bokeh\_2021\\2021\_08\_25\_Bokeh\_2021\\2021\_08\_25\_Bokeh\_2021\\2021\_08\_25\_Bokeh\_2021\\2021\_08\_25\_Bokeh\_2021\\2021\_08\_25\_Bokeh\_2021)
3 Configurational Setting of Tersoff Potential

The Tersoff potential belongs to the class of empirical-analytical bond order interatomic potentials, having the advantage of approximating chemical reactions as well as describing different bonding states of an atom. The Tersoff potential includes two-body and three-body interactions rendering pair and triplet terms, respectively. Our configurational formulation accounts for the release of total potential energy due to the pair length and triplet area changes. Thus, we initially introduce the configurational Tersoff potential density, as follows:

The total potential energy of a system composed of a finite number of atoms interacting mutually is described as the sum of interatomic potential densities

\[ E = \frac{1}{6} \sum_{\gamma \neq \beta \neq \alpha} W^t_{\alpha\beta}(\Lambda_{\alpha\beta}, \Lambda_{\alpha\gamma}, \Lambda_{\beta\gamma}, P_{\alpha\beta\gamma}), \]  

(14)

where we reformulate the bonding energy of Tersoff as,

\[ W^t_{\alpha\beta} = W^t_c(\Lambda_{\alpha\beta}) \left[ W^t_R(\Lambda_{\alpha\beta}) x_{\alpha\beta} + W^t_P(\Lambda_{\alpha\beta}) a_{\alpha\beta} W^t_A(\Lambda_{\alpha\beta}) x_{\alpha\gamma} \right] \]  

(15)

A smooth configurational cut-off function is defined using pair stretch, it limits the interatomic interactions to the first-nearest neighbor. The function takes the form,

\[ W^t_c(\Lambda_{\alpha\beta}) = \begin{cases} 
1, \\
\frac{1}{2} \left[ 1 - \sin \left( \frac{\pi}{2} \frac{1-R^0(\Lambda_{\alpha\beta})}{D^0(\Lambda_{\alpha\beta})} \right) \right], & \frac{1}{R^0(\Lambda_{\alpha\beta})} \leq \Lambda_{\alpha\beta} \leq \frac{1}{R^0(\Lambda_{\alpha\beta}) + D^0(\Lambda_{\alpha\beta})} \\
0, & \Lambda_{\alpha\beta} \leq \frac{1}{R^0(\Lambda_{\alpha\beta})}. 
\end{cases} \]  

(16)

The range of interaction can be adjusted based on the parameters \( R^0 \) and \( D^0 \), presenting the interaction radius. The value of the cut-off function in this range smoothly reduces from 1 to 0. Repulsive and attractive interactions between atoms, rendering pair-wise potentials, are defined as potential densities of Morse-type interaction as

\[ W^t_R(\Lambda_{\alpha\beta}) = A^0 \Lambda_{\alpha\beta} \exp \left( -\frac{\lambda^0_1}{\Lambda_{\alpha\beta}} \right) \]  

(17)

\[ W^t_A(\Lambda_{\alpha\beta}) = -B^0 \Lambda_{\alpha\beta} \exp \left( -\frac{\lambda^0_2}{\Lambda_{\alpha\beta}} \right) \]  

(18)

The Tersoff potential includes a three-body interaction, such that the interaction between a system of three atoms can be defined using the cosine map of the angle between them. Using such a term, the influence of the local environment of every individual atom is considered. We define the configurational triplet potential density as a function of pair and triplet stretches,

\[ W^t_{\phi} = \left[ 1 + \beta^0 c_{n_{\alpha\beta\gamma}} \right]^{-1/2} \]  

(19)

\[ \zeta^m_{\alpha\beta\gamma} = d_0 P_{\alpha\beta\gamma} \sum_{\gamma \neq \alpha, \beta} W^t_c(\Lambda_{\alpha\beta\gamma}) g^t(\Omega_{\alpha\beta\gamma}) \exp \left( (\lambda^0_3 |\alpha\gamma - \Lambda_{\alpha\beta\gamma}|)^m \right), \]  

(20)

with the triplet twist potential density using the material twist,

\[ g^t(\Omega_{\alpha\beta\gamma}) = \eta^0_{\alpha\beta\gamma} \Omega_{\alpha\beta\gamma} \left[ 1 + \frac{c^2}{d^2} - \frac{c^2}{d^2} \left( \frac{1}{\Omega^2_{\alpha\beta\gamma}} - \frac{1}{\omega^0_{\alpha\beta\gamma}} - \omega^0_{\alpha\beta\gamma} \right) \right]. \]  

(21)

We redefine the coefficients of the Tersoff potential as presented in Table. 1 to provide a unit for potentials as energy per unit of spatial length or area.

| \( R^0 \) | \( D^0 \) | \( A^0 \) | \( B^0 \) | \( d_0 \) |
|---|---|---|---|---|
| \( R/\lambda_{1\alpha\beta} \) | \( D/\lambda_{1\alpha\beta} \) | \( A/\lambda_{1\alpha\beta} \) | \( B/\lambda_{1\alpha\beta} \) | \( 1/\lambda_{1\alpha\beta} \) |

| \( \lambda^0_1 \) | \( \lambda^0_2 \) | \( \lambda^0_3 \) | \( \eta^0_{\alpha\beta\gamma} \) | \( \omega^0_{\alpha\beta\gamma} \) |
|---|---|---|---|---|
| \( \lambda_1 X_{\alpha\beta} \) | \( \lambda_2 X_{\alpha\beta} \) | \( \lambda_3 X_{\alpha\beta} X_{\alpha\gamma} \) | \( \eta_{\alpha\beta\gamma} \Theta_{\alpha\beta\gamma} \) | \( \cos \theta_{\alpha\beta\gamma} \) |

Table 1: Table of coefficients in configurational Tersoff potential.

In the following we derive configurational forces for the case that spatial positions of atoms are fixed, however the material positions can vary, i.e., \( d_\delta X_\gamma \). The material variations of the total potential energy \( E \) is denoted as virtual energy release, \( R_\delta \).

That is,

\[ R_\delta := d_\delta E \leq 0 \quad \forall d_\delta \{X_\gamma\}. \]  

(22)
Due to the dependency of external potential energy merely on spatial atomistic positions, we do not observe energy release associated with the changes in external energy. We derive configurational forces as the thermodynamic conjugate of configurational changes, thus we define configurational pair forces as the cluster sum of interatomic pair configurational forces,
\[
\mathbf{K}_{\alpha}^{\text{pair}} = \frac{1}{2!} \sum_{\beta \neq \alpha} \mathbb{K}_{\alpha \beta}, \quad \text{where,} \quad \mathbb{K}_{\alpha \beta} := \left[ \partial_{\Lambda_{\alpha \beta}} W_{R}^{t} + \partial_{\Lambda_{\alpha \beta}} W_{A}^{t} \right] N_{\alpha \beta}.
\tag{23}
\]
In addition, configurational triplet forces are derived as the sum of interatomic triplet configurational forces,
\[
\mathbf{K}_{\alpha}^{\text{triplet}} = \frac{1}{3!} \sum_{\gamma \neq \beta \neq \alpha} \mathbb{K}_{\alpha \beta \gamma}, \quad \text{considering,} \quad \mathbb{K}_{\alpha \beta \gamma} := \partial_{P_{\alpha \beta \gamma}} W_{\theta}^{t} N_{\alpha \beta \gamma}.
\tag{24}
\]
Further more, we carry out a molecular statics study on a mono-layer pre-cracked graphene sheet at zero Kelvin by size $42.66 \times 135.66$ Å$^2$ including 2200 carbon atoms. A Mode-I loading as a total displacement of 5.6 Å in 70 steps is applied to the pink atoms. Each displacement is followed by the minimization of total potential energy to obtain deformed lattice. The Tersoff potential models the lattice and allows us to examine the influence of pair stretch and triplet twist in the release of total energy. Figure 2 (a) illustrates the deformation graphene in step 60 under the total displacement of 4.8 Å. We observe that configurational pair forces (blue arrays) appear at the vicinity of the pre-crack, while they also identify free and constrained edges. Dislocation emission under the deformation causes the material evolution. The material evolution is captured by the emergence of configurational forces (Fig. 2 (b)), rendering energy release due to material length and area changes (Fig. 2 (d)). It is also presented in [5] that configurational forces can be used as a criterion for re-organization (evolution) of material numerically. Finally, Figure 2 (c) illustrates the displacement-deflection curve of the mono-layer lattice indicating the failure at displacement step 60.

![Fig. 2](image_url)

Fig. 2: a presents the spatial configuration including the emission of dislocations from crack tip. b depicts that the emission path is precisely captured by configurational forces, rendering the released energy due to the defect evolution in d. c demonstrates the displacement-deflection curve of mono-layer graphene.

4 Conclusion and discussion

In this work, we elaborated configurational mechanics of the bond order Tersoff potential to introduce the atomistic configurational pair and triplet forces, capturing the stretches in the two-body length and the three-body area during deformation. The application of atomistic configurational forces is assessed in a pre-cracked graphene sheet. We observed that configurational forces trace the defect evolution into the lattice as well as rendering release of total energy.

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