On the Modified Virtual Internal Bond Method

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The virtual internal bond (VIB) method was developed for the numerical simulation of fracture processes. In contrast to the traditional approach of fracture mechanics where stress analysis is separated from a description of the actual process of material failure, the VIB method naturally allows for crack nucleation, branching, kinking, and arrest. The idea of the method is to use atomic-like bond potentials in combination with the Cauchy-Born rule for establishing continuum constitutive equations which allow for the material separation–strain localization. While the conventional VIB formulation stimulated successful computational studies with applications to structural and biological materials, it suffers from the following theoretical inconsistency. When the constitutive relations of the VIB model are linearized for an isotropic homogeneous material, the Poisson ratio is found equal to 1/4 so that there is only one independent elastic constant—Young's modulus. Such restriction is not suitable for many materials. In this paper, we propose a modified VIB (MVIB) formulation, which allows for two independent linear elastic constants. It is also argued that the discrepancy of the conventional formulation is a result of using only two-body interaction potentials in the microstructural setting of the VIB method. When many-body interactions in "bond bending" are accounted for, as in the MVIB approach, the resulting formulation becomes consistent with the classical theory of isotropic linear elasticity.
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1 Introduction

As a possible alternative to the Griffith-Orowan-Irwin approach to fracture mechanics, multiscale material considerations may be used to formulate continuum models allowing for material separation–strain localization. Based on the so-called Cauchy-Born rule, a virtual internal bond approach to modeling material failure has been proposed by Gao and Klein [1]. This approach differs from atomistic methods in that a phenomenological "cohesive force law" is assumed to act between "material particles" which are not necessarily atoms; it also differs from the "cohesive surface" models in that, rather than imposing a cohesive law along a prescribed set of discrete surfaces, a network of cohesive bonds is statistically incorporated into a constitutive law via the Cauchy-Born rule, i.e., by equating the strain energy density on the continuum level to the potential energy stored in the cohesive bonds due to the imposed deformation.

Although the conventional formulation of the VIB model can be successfully used in simulations of crack nucleation, growth, kinking, and branching, it suffers from the following inconsis-

tency. When the constitutive relations of the VIB model are linearized for an isotropic homogeneous material, they allow for only one independent material constant—Young's modulus—while the second constant—Poisson ratio—is not independent and it is equal to 1/4. Since such restriction is not suitable for many materials, it is desirable to modify the conventional VIB formulation. This is done in the present work. The modified formulation allows for two independent material constants in the case of the linearized isotropic elasticity. The conventional formulation of VIB is based on two-body interaction potentials in the microstructural setting. The modified VIB approach accounts for many-body interactions associated with "bond bending" and the resulting formulation appears to be more consistent with the classical theory of isotropic linear elasticity.

2 Conventional VIB Formulation and its Deficiency

Consider a solid body comprising microparticles, for example, atoms, placed at $\mathbf{r}_i$ in the 3D space. Generally, the volumetric density of the total potential energy of the body is a function of the particle positions: $\Phi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_n)$, where n is the number of particles. More specifically, the potential energy can be written in terms of two-particle interactions as

$$\Phi = \frac{1}{2\Omega} \sum_{i,j} U(r_{ij}), \quad r_{ij} = |\mathbf{r}_{ij}| = |\mathbf{r}_i - \mathbf{r}_j|, \qquad (2.1)$$

where Ω is the volume occupied by the system.

According to the Cauchy-Born rule, originally applied to the crystal elasticity, the current $\mathbf{r}_{ij}$ and initial (reference) $\mathbf{R}_{ij} = \mathbf{R}_i - \mathbf{R}_j$ relative positions of the same two particles can be related by the deformation gradient $\mathbf{F} = \mathrm{Grad}\,\chi(\mathbf{X})$:

$$\mathbf{r}_{ij} = \mathbf{F}\mathbf{R}_{ij}, \qquad (2.2)$$

It is assumed above that particles are in the vicinity of point $\mathbf{X}$ at the reference state. This point is placed at $\chi(\mathbf{X})$ after the deformation.

Substituting Eq. (2.2) in Eq. (2.1) yields

$$\Phi = \frac{1}{2\Omega} \sum_{i,j} U(r_{ij}) = \Phi(\mathbf{C}), \quad \mathbf{C} = \mathbf{F}^T\mathbf{F}. \qquad (2.3)$$

Now the second Piola-Kirchhoff stress tensor and the tangent stiffness, moduli can be derived in the usual way: $S_{IJ} = 2\partial\Phi/\partial C_{IJ}$; $K_{IJMN} = 2\partial S_{IJ}/\partial C_{MN}$. Evidently, the microstructural approach is as phenomenological as continuum mechanics. The phenomenology, however, is moved to the microlevel in the former case to allow for more flexible analysis.

Direct application of Eq. (2.3) to analysis of material behavior seems to be difficult because of the large amount of microparticles. Gao and Klein [1] and Klein and Gao [2,3] proposed the following averaging procedure:

$$\Phi = \frac{1}{\Omega_0} \int_{\Omega_0^*} U(l)D_\Omega d\Omega. \qquad (2.4)$$

Here Ω_0 is the reference representative volume; $U(l)$ is the bond potential; $l = r_{ij} = L\sqrt{\xi_I C_{IJ}\xi_J}$ is the current virtual bond length; $\boldsymbol{\xi} = (\mathbf{R}_i - \mathbf{R}_j)/L$; $L = R_{ij} = |\mathbf{R}_i - \mathbf{R}_j|$; D_Ω is the volumetric bond density function; and Ω_0^* is the integration volume defined by the range of influence of U.

Considerations being limited to centrosymmetric bond density functions, where spherical coordinates are used: $\xi_1 = \sin\theta\cos\varphi$; $\xi_2 = \sin\theta\sin\varphi$; $\xi_3 = \cos\theta$, it is possible to express an average as

$$\langle\bullet\rangle = \frac{1}{\Omega_0} \int_{-\pi}^{\pi} \int_0^\pi \int_0^{L^*} (\bullet)D(L,\theta,\varphi)L^2 \sin\theta dLd\theta d\varphi, \quad (2.5)$$

where L^* presents the maximum distance over which particles interact. Then the elastic moduli take the form

$$K_{IJMN} = 4\partial\Phi/\partial C_{IJ}\partial C_{MN} = \langle(U''(l)/l^2 - U'(l)/l^3)L^4\xi_I\xi_J\xi_M\xi_N\rangle.$$

(2.6)

The precise definition of $D(L,\theta,\varphi)$ is that $D(L,\theta,\varphi)L^2\sin\theta dLd\theta d\varphi$ presents the number of bonds in the undeformed solid with bond length between L and $L+dL$ and orientation between $\{\theta,\varphi\}$ and $\{\theta+d\theta,\varphi+d\varphi\}$.

So far, most reported analyses based on the VIB model use the simple two-parameter phenomenological cohesive force law: $U'(l)=A(l-L)\exp[-B(l-L)]$, where A is the slope of $U'(l)$ for the unstretched bond and $1/B$ is the critical stretch at which the maximum bond strength is reached.

The deficiency of the conventional formulation appears under the assumption of homogeneity and isotropy of material, i.e., $D(L,\theta,\varphi)=D_L(L)$. In this case, the linearized elastic moduli take the form

$$K_{IJMN} = \langle U''(L)L^2\rangle_L \int_{-\pi}^{\pi}\int_0^{\pi}\xi_I\xi_J\xi_M\xi_N\sin\theta d\theta d\varphi$$

$$= \mu(\delta_{IJ}\delta_{MN} + \delta_{IM}\delta_{JN} + \delta_{IN}\delta_{JM}).$$

(2.7)

Here $\mu=4\pi\langle L^2 U''(L)\rangle_L/15$ is the only elastic (Lame) constant. The latter is in contradiction with the continuum mechanics result for isotropic linear materials, which should have two independent material constants. We can compare this tensor of elastic moduli to the classical isotropic linear elasticity. In the latter case, the elastic moduli tensor takes the following form,

$$H_{IJMN} = \lambda\delta_{IJ}\delta_{MN} + \mu(\delta_{IM}\delta_{JN} + \delta_{IN}\delta_{JM}),$$

(2.8)

where $\lambda=2\mu\nu/(1-2\nu)$ is the second Lame constant and ν is the Poisson ratio. By setting $\nu=1/4$ we obtain $\lambda=\mu$ and $H_{IJMN}=K_{IJMN}$. Thus the VIB formulation allows for the linear isotropic elasticity as a special case where the Poisson ratio equals $1/4$. Since this restriction is not suitable for the description of many materials, we propose a modification of the VIB method to be fully consistent with the classical linear elasticity.

3 Modified VIB Formulation

The simple pair (two-body) potential used within the Cauchy-Born approach is a good candidate to be responsible for the inconsistencies of the conventional VIB model[1] pointed out above. It seems that the role of the averaging procedure is fairly subsidiary in the inconsistencies of the whole approach. Modification of the cohesive law and the use of a different analytical expression instead of the exponential law, say the Lennard-Jones potential, will not help if the cohesive law does not change qualitatively. We discuss one way to revise and modify the conventional VIB approach below.

From the microstructural point of view, the simple pair potential does not allow for considering simultaneous multiple (multibody) particle interactions.[2] It may be said, instead, following Phillips and Ortiz [4], that the pair potential excludes "bending" of the bonds between the particles. A way to circumvent this problem and to include bending of the bonds in analysis is to extend Eq. (2.1) to the three-body terms, for example,

$$\Phi = \frac{1}{2\Omega}\sum_{i,j}U(r_{ij}) + \frac{1}{3!\Omega}\sum_{i,j,k}V(r_{ij},r_{jk},\vartheta_{ijk}),$$

(3.1)

where ϑ_{ijk} is an angle between $\mathbf{r}_k-\mathbf{r}_j$ and $\mathbf{r}_i-\mathbf{r}_j$, and V is, say, the Stillinger-Weber [5] potential. The number of simultaneously interacting particles can be further increased, of course. In the latter

case, it is not entirely clear where this process should be truncated and what the multi-body potentials should look like. We proceed with a different plan (see [6]), which should be preceded by the following methodological remark.

The Cauchy-Born approach is a mixture of atomistic, or particulate, and continuum concepts. The weight of the atomistic concepts in setting the approximate material model is dominant when one plays with the number of interacting particles and the character of their interaction. The concept of continuum deformation appears only at the last stage of the model formulation when Eq. (2.2) is used. Below, we propose a different strategy where the character of continuum deformation—dilatation/distortion—is essentially involved in the model formulation while the potential energy includes only two-body interactions, in which the pairbonds enjoy both stretching and bending.

From the point of view of continuum mechanics, we begin with replacing the interatomic distance r_{ij} in the total potential energy by a more convenient quadratic measure of the interatomic distance change

$$\Delta = l^2 - L^2 = L^2(C_{IJ} - \delta_{IJ})\xi_I\xi_J = 2L^2 E_{IJ}\xi_I\xi_J,$$

(3.2)

where $\mathbf{E}=(\mathbf{C}-\mathbf{1})/2$ is the Green strain tensor. Let this tensor be decomposed into spherical and deviatoric parts accordingly:

$$E_{IJ} = E_{KK}\delta_{IJ}/3 + \hat{E}_{IJ}.$$

(3.3)

Substituting Eq. (3.3) in Eq. (3.2) we have

$$\Delta = \psi + \hat{\Delta}, \quad \psi = 2L^2 E_{KK}/3, \quad \hat{\Delta} = 2L^2\hat{E}_{IJ}\xi_I\xi_J.$$

(3.4)

Here ψ is the bond length change due to spherical dilatational deformation and $\hat{\Delta}$ is the bond length change due to the devitoric deformation.

Now the stored energy can be written in the following form:

$$U(\Delta) = U(\psi,\hat{\Delta}) = A - A(1 + \psi\sqrt{B/A})\exp[-\psi\sqrt{B/A} - \hat{\Delta}^2 C/(2A)].$$

(3.5)

The physical meaning of the introduced potential can be clarified with the help of the "stretching" and "shearing" forces which are derived by differentiating the potential with respect to ψ and $\hat{\Delta}$ accordingly:

$$U_\psi = \frac{\partial U(\psi,\hat{\Delta})}{\partial\psi} = B\psi\exp[-\psi\sqrt{B/A} - \hat{\Delta}^2 C/(2A)],$$

(3.6)

$$U_{\hat{\Delta}} = \frac{\partial U(\psi,\hat{\Delta})}{\partial\hat{\Delta}} = C(1 + \psi\sqrt{B/A})\hat{\Delta}\exp[-\psi\sqrt{B/A} - \hat{\Delta}^2 C/(2A)].$$

(3.7)

These forces are presented in Fig. 1. The maximum of U_ψ occurs at $\psi=\sqrt{A/B}$, where $\hat{\Delta}=0$. B is the slope of U_ψ at $\psi=0$. The maximum of $U_{\hat{\Delta}}$ occurs at $\hat{\Delta}=\pm\sqrt{A/C}$, where $\psi=0$. C is the slope of $U_{\hat{\Delta}}$ at $\hat{\Delta}=0$.

In order to examine consistency of the modified VIB formulation with the linear elasticity, we compute the linearized tensor of elastic moduli for isotropic materials. Omitting tedious intermediate transformations we get finally

$$K_{IJMN} = \langle L^4\rangle_L\pi\left(\frac{16}{9}B - \frac{32}{45}C\right)\delta_{IJ}\delta_{MN} + \langle L^4\rangle_L\pi\frac{16}{15}C(\delta_{IM}\delta_{JN} + \delta_{IN}\delta_{JM}),$$

(3.8)

Comparing Eq. (3.8) with the elastic moduli of the classical linear theory [Eq. (2.8)] we obtain for the Lame parameters

$$\lambda = \pi\langle L^4\rangle_L\left(\frac{16}{9}B - \frac{32}{45}C\right), \quad \mu = \pi\langle L^4\rangle_L\frac{16}{15}C.$$

(3.9)

These two formulas present the relations between the macroscopic Lame parameters and the microscopic parameters of the bond potential.

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[1]Klein and Gao [2] extended the VIB method to directionally bonded lattices such as Si by introducing an internal degree of freedom. This approach is not applicable to the isotropic case.

[2]Here we mean a simultaneous interaction of many particles, which cannot be described by a sum of the pair potentials of every two particles involved in the interaction as it is often done in the literature.
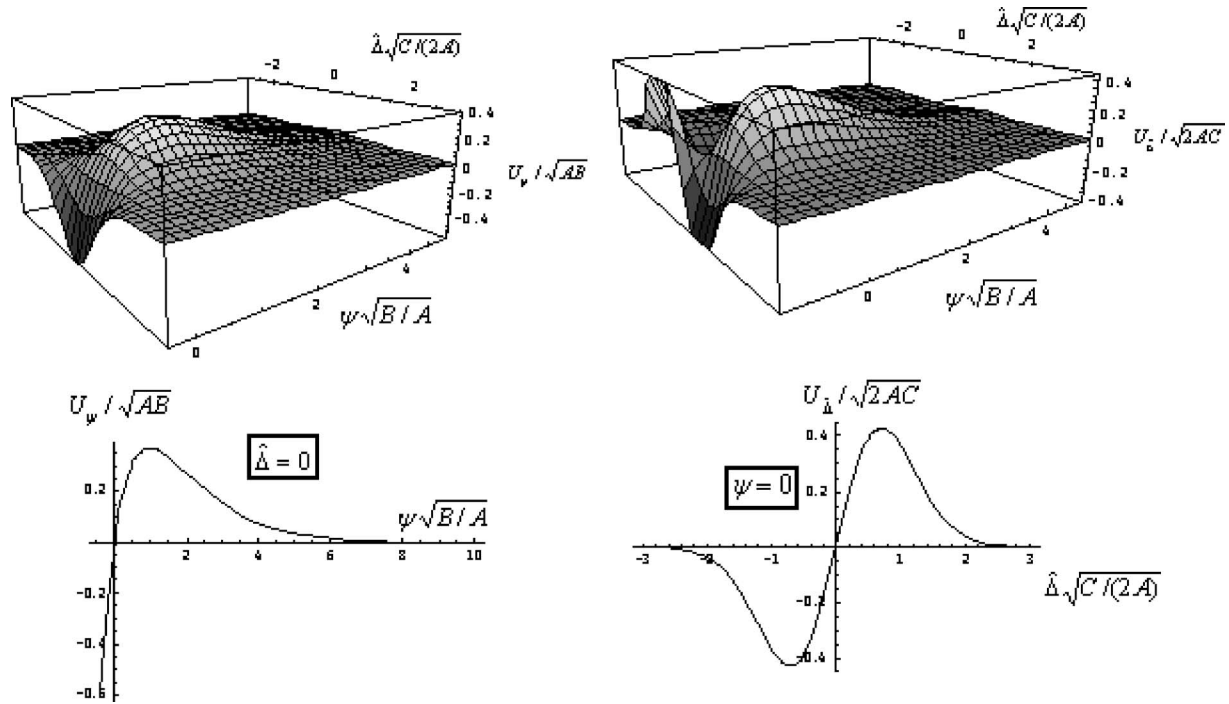
Fig. 1 "Stretching" (left) and "shearing" (right) forces in the modified VIB formulation

4 Concluding Remarks

A modified formulation of the virtual internal bond method has been proposed in the present work. At the level of material particles or atoms, this formulation still considers two-body (pair) bonds. However, these bonds possess both stretching and bending stiffness. The stretching stiffness corresponds to the classical interaction of two particles along the line connecting them. The bending stiffness of the bond is a more subtle subject. It is supposed to account for the simultaneous interactions between the given two particles and other particles (multi-body interaction) without explicitly introducing the latter ones. The modified VIB (MVIB) formulation resolves the discrepancy between the conventional VIB formulation and the classical linear elasticity because the MVIB formulation leads to two independent material parameters. The latter is in contrast to the conventional VIB formulation which leads to only one independent material parameter when it is linearized. Thus the conventional VIB formulation is not in peace with the well-established classical theory of isotropic elasticity which requires two independent material parameters.

The modified VIB formulation is a marriage of the conventional VIB formulation and the purely phenomenological approach of Volokh [6]. While the differences between the conventional and modified VIB formulations are clear from the present work, the qualitative comparison between MVIB and the phenomenological approach is worth performing. The advantages of the MVIB method come from its intrinsic consideration of the material microstructure. Particularly, the MVIB approach naturally allows for considering material anisotropy and introducing the characteristic length scale. These features make the MVIB method physically desirable and more flexible than the phenomenological framework of Volokh [6]. On the other hand, the MVIB formulation is more involved computationally and this is the expected price for its generality.

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