Orientation Element Based Constitutive Model and Lattice Model

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Abstract A general formulation of the Helmholtz free energy used in thermodynamics is derived within the framework of the embedded-atom method with the Cauchy-Born rule. Such a physics-based thermodynamic state potential does not directly incorporate the interatomic potentials and atomic structure of a material, but subsumes the statistical ensemble average of the action of the entirety of microscopic degrees of freedom. The constitutive behavior of a non-dissipative material is therefore entirely determined by this free energy, and is not subject to length and time scale limitations. Moreover, it is proved that the contribution of the two-body potential to the free energy is expressed as the integral of potentials defined in different orientation over the hemisphere, and individual potential in each orientation yields 1D constitutive law. Consequently, the discretization of the integration furnishes a unified framework for the development of the truss lattice models for computational micromechanics, as well as of the truss-type lattice structured materials in engineering applications.

Key words: Cauchy-Born rule, free energy, constitutive model, discretization, lattice model

INTRODUCTION

The constitutive equation that relates the forces within a solid and the deformations that attend them is one of the most important properties of material behavior. Modern industry requires higher credibility and nicety of the used structures. There is a need for development and ceaselessly more improvement of the constitutive relation of solid material with the help of the theory of mechanics, advanced computers and experimental techniques. Broadly speaking, the determination of the constitutive relation is based on two fundamental physical models: discrete atomic models and continuum models.

Since the descriptions by a discrete atomic model and by a continuum model are independent and thoroughly different, one of fundamental questions faced in the construction of realistic and tractable constitutive models is how best to reconcile atomic descriptions, which are presumed to represent the true mechanic underpinning of a given process, and continuum descriptions, whose aim is to capture the essential physics of a particular process, and to use this reduced description as a predictive tool. Thereby, the so-called Cauchy-Born rule (CBR) has been applied, which represents atomic coordinates in the current deformed configuration as affine mapping of the atomic coordinates in the reference configuration in terms of the local deformation gradient of the continuum [1, 2]. Within the framework of hyperelasticity with the CRB, the overall properties of a solid can be obtained by equating the deformation energy of a continuum material particle to that of the underlying assemble of atoms due to an imposed deformation. Since the interatomic interactions are directly incorporated into the constitutive model of the solid and additional phenomenological input is circumvented, such a continuum-atomic theory has been used to model the multiscale problem involving atoms and continua [3, 4].

The purpose of the current paper is, on one hand, to formulate the Helmholtz free energy used in thermodynamics within the framework of the embedded-atom method [5] with the Cauchy-Born rule, and then to construct the orientation element based constitutive model (OEBCM) for non-dissipative materials. On the other hand, we discuss the numerical implementation of the OEBCM. The truss lattice model [6], which offers an attractive alternative to finite element analysis of materials, is directly derived from the discretization of the OEBCM. Finally, the optimum design of as well as the investigation of the effective

mechanical properties of the truss-type lattice structured materials [7] can also be cased into the framework of the discretization of the OEBCM.

ORIENTATION ELEMENT BASED CONSTITUTIVE MODEL

1. Construction of thermodynamic state potential Consider a solid material consisting of continuum material particles at the macroscopic scale, in which the deformation within an infinitesimal neighborhood of a material particle is regarded as uniform. On the atomic scale, the infinitesimal material neighborhood is associated to a representative ensemble of atoms with sufficient large number of atoms. Denote the reference configuration of the assemble of atoms by A and the current deformed configuration by B. The distance vectors between two atoms α and β, i.e. $R^{(\alpha,\beta)}$ and $r^{(\alpha,\beta)}$ in configuration A and in configuration B is then written as, respectively

$$R^{(\alpha,\beta)} = R^{(\alpha)} - R^{(\beta)}, \ r^{(\alpha,\beta)} = r^{(\alpha)} - r^{(\beta)} \ \text{with} \ R^{(\alpha,\beta)} = \left| R^{(\alpha,\beta)} \right|, \ r^{(\alpha,\beta)} = \left| r^{(\alpha,\beta)} \right| \tag{1}$$

Following the CBR, it is assumed that the coordinate of atom α, $R^{(\alpha)}$, in configuration A is deformed into the coordinate $r^{(\alpha)}$ in configuration B by the deformation gradient F of the infinitesimal neighborhood,

$$r^{(\alpha)} = F \cdot R^{(\alpha)} \tag{2}$$

The Green strain ε is defined by

$$\varepsilon = \frac{1}{2}(F^T \otimes F - I) \tag{3}$$

where I is the second order identity tensor (Kronecker delta symbol). From Eqs. (1), (2) and (3), one can easily see that in configuration B the distance between two atoms α and β

$$r^{(\alpha,\beta)} = R^{(\alpha,\beta)}\sqrt{2\varepsilon : (N^{(\alpha,\beta)} \otimes N^{(\alpha,\beta)}) + 1} \tag{4}$$

where $N^{(\alpha,\beta)}$ is the unit vector of $R^{(\alpha,\beta)}$.

When the deformations of the continuum and the representative ensemble of atoms are linked via the CBR under isothermal conditions, the continuum energy density per unit volume can be calculated exclusively from the interatomic potential energy density of underlying atoms and the macroscopic strain, and do not involve empirical phenomenological assumption. Within the framework of the embedded-atom method [5], the energy density of the representative ensemble of atoms takes the form

$$e = \frac{1}{2V}\sum_{\alpha,\beta(\alpha\neq\beta)}\phi(r^{(\alpha,\beta)}) + \frac{1}{V}\sum_{\alpha}\psi^{(\alpha)}(\rho^{(\alpha)}) \tag{5}$$

Here V is the volume of the assemble of atoms; the indices α and β run over all atoms in the representative ensemble of atoms; $\phi(r^{(\alpha,\beta)})$ is the two-body potential related to a specified pair of atoms α and β with the distance $r^{(\alpha,\beta)}$; $\psi^{(\alpha)}(\rho^{(\alpha)})$ is the energy required to embed atom α into the background electron density $\rho^{(\alpha)}$. The electron density at atom α is approximated as the supposition of the electron densities due to the surrounding atoms at the location of atom α

$$\rho^{(\alpha)} = \sum_{\beta(\neq\alpha)} f(r^{(\alpha,\beta)}) \tag{6}$$

where $f(r^{(\alpha,\beta)})$ is the electron density generated by atom β at a distance $r^{(\alpha,\beta)}$ from its core.

Despite the virtues inherent in the incorporation of the interatomic potentials and atomic structure of a material into the continuum energy density, direct atomic calculation on realistic time scale and structures is still not feasible, and is often excessive and unnecessary. We are therefore attempting to replace the pair functional setting in Eq. (5) by those approximate surrogates. The latter removes the atomic-level degrees of freedom, but subsumes the statistical ensemble average of the action of the entirety of microscopic degrees of freedom. For that, select a spherical coordinate system (R,θ,φ) so that the distance vector between two atoms in configuration A is characterized by a position in the upper half spherical coordinate

system (considering the potential energy density is independent of the orientation of the distance vectors, herein we require all atomic distance vectors to be oriented in the upper half spherical coordinate system). Because the number of atoms is sufficiently large, the maximum distance over which atoms interact in configuration A can be conceived as be infinite.

The discrete summation expression of the first item on the right-hand side of Eq. (5) can then be linked into the continuous integral form by

$$\frac{1}{2V}\sum_{\alpha,\beta(\alpha\neq\beta)}\phi(r^{(\alpha,\beta)})=\frac{1}{2}\int_0^{2\pi}\int_0^{\pi/2}\int_0^\infty D(R,\theta,\varphi)\phi(R\sqrt{2\varepsilon:(N\otimes N)+1})\sin\varphi dRd\theta d\varphi \tag{7}$$

Here $D(R,\theta,\varphi)$ is the distribution function of the positions located by the distance vectors in the hemispherical space, and is given by

$$D(R,\theta,\varphi)=\sum_I\sum_J\sum_K\frac{M(R^{(I)},\theta^{(J)},\varphi^{(K)})}{2V\sin\varphi}\delta(R-R^{(I)})\delta(\theta-\theta^{(J)})\delta(\varphi-\varphi^{(K)}) \tag{8}$$

where I, J and K run over all the positions located by the distance vectors in the spherical coordinate system, respectively, $M(R^{(I)},\theta^{(J)},\varphi^{(K)})$ is the number of the distance vectors locating at site $(R^{(I)},\theta^{(J)},\varphi^{(K)})$, δ is the Dirac delta function. In the spherical coordinates N_i is represented as

$$N_1=\sin\varphi\cos\theta, \qquad N_2=\sin\varphi\sin\theta, \quad N_3=\cos\varphi \tag{9}$$

Defining the energy function in the direction (θ,φ)

$$\Phi(\theta,\varphi,\varepsilon:(N\otimes N))=\frac{\pi}{15}\int_0^\infty D(R,\theta,\varphi)\phi(R\sqrt{2\varepsilon:(N\otimes N)+1})dR \tag{10}$$

and bringing it into Eq. (7), the contribution of the two-body potential to the continuum energy density can be written as the integral of the energy functions defined in different directions,

$$\frac{1}{2V}\sum_{\alpha,\beta(\alpha\neq\beta)}\phi(r^{(\alpha,\beta)})=\frac{15}{2\pi}\int_0^{2\pi}\int_0^{\pi/2}\Phi(\theta,\varphi,\varepsilon:(N\otimes N))\sin\varphi d\theta d\varphi \tag{11}$$

Similarly, the distribution function of the positions located by the distance vectors between atom α and all other atoms in the above hemispherical space can be given by

$$\overline{D}^{(\alpha)}(R,\theta,\varphi)=\sum_{I^{(\alpha)}}\sum_{J^{(\alpha)}}\sum_{K^{(\alpha)}}\frac{1}{\sin\varphi}\delta(R-R^{(I^{(\alpha)})})\delta(\theta-\theta^{(J^{(\alpha)})})\delta(\varphi-\varphi^{(K^{(\alpha)})}) \tag{12}$$

where $I^{(\alpha)}$, $J^{(\alpha)}$ and $K^{(\alpha)}$ run over all the positions located by the distance vectors between atom α and other atoms in the hemispherical space, respectively. Substitution of Eq. (12) into Eq. (6) yields

$$\rho^{(\alpha)}=\int_0^{2\pi}\int_0^{\pi/2}\int_0^\infty \overline{D}(R,\theta,\varphi)f(R\sqrt{2\varepsilon:(N\otimes N)+1})\sin\varphi dRd\theta d\varphi \tag{13}$$

By expanding f into a Taylor series with respect to ε and neglecting terms of order two and higher, we get

$$f(R\sqrt{2\varepsilon:(N\otimes N)+1})\approx f(R)+f'(R)R(\varepsilon:(N\otimes N)) \tag{14}$$

By substituting Eq. (14) into Eq. (13) and making use of the relation

$$\int_0^{2\pi}\int_0^{\pi/2}N\otimes Nd\theta d\varphi=\frac{2\pi}{3}I \tag{15}$$

$\rho^{(\alpha)}$ can approximately written as

$$\rho^{(\alpha)}\approx\rho_0^{(\alpha)}(1+\chi^{(\alpha)}\varepsilon:I) \tag{16}$$

where $\rho_0^{(\alpha)}$ and $\chi^{(\alpha)}$ are two constants. Bringing Eq. (16) into Eq. (5), the contribution of the embedding

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energy of atoms to the continuum energy density can be expressed by the energy function

$$\Psi(\boldsymbol{\varepsilon}:\boldsymbol{I}) = \frac{1}{V}\sum_\alpha \psi^{(\alpha)}(\rho_0^{(\alpha)}(1+\chi^{(\alpha)}\boldsymbol{\varepsilon}:\boldsymbol{I})) \tag{17}$$

The definition of two types of energy functions in Eqs. (11) and (17) provides a physical basis for the construction of thermodynamic state potential (the Helmholtz free energy) used in thermodynamics. The total free energy per unit volume is written as a sum of two independent parts: an atomic part and an electronic part, corresponding to the self-interaction of the nuclei as well as effective interaction between the nuclei and surrounding electron gas in the system, respectively

$$e(\boldsymbol{\varepsilon}) = \frac{15}{2\pi}\int_\Omega \Phi_\Omega(\varepsilon_N)d\Omega + \Psi(\varepsilon_V) \tag{18}$$

where the integral domain represented by Ω represents the upper half hemisphere, the expressions of the normal and volumetric strains ε_N and ε_V are

$$\varepsilon_N = \boldsymbol{\varepsilon}:(\boldsymbol{N}\otimes\boldsymbol{N}), \qquad \varepsilon_V = \boldsymbol{\varepsilon}:\boldsymbol{I} \tag{19a,b}$$

2. Constitutive law of non-dissipative materials For non-dissipative (thermoelastic) materials, Fung [8] provides an classification of the different forms of elastic model. Within his classification the formulation requires all materials to be hyperelastic, since this is the only means by which the material is guaranteed to obey the First Law of Thermodynamics.

The behavior of a hyperelastic material is entirely defined by a Helmholtz free energy function. In view of an isothermal deformation process, a physics-based hyperelastic constitutive law can be obtained by virtue of the free energy derived in Eq. (18). Making use of Eqs. (19ab), the symmetric (second) Piola-Kitchhoff stress tensor is defined by

$$\sigma_{ij} = \frac{\partial e}{\partial \varepsilon_{ij}} = \frac{15}{2\pi}\int_\Omega \frac{\partial \Phi_\Omega(\varepsilon_N)}{\partial \varepsilon_N}N_i N_j d\Omega + \frac{\partial \Psi(\varepsilon_V)}{\partial \varepsilon_V}\delta_{ij} \tag{20}$$

and the tangent stiffness tensor obtained by further differentiation

$$C_{ijst} = \frac{\partial^2 e}{\partial \varepsilon_{ij}\partial \varepsilon_{st}} = \frac{15}{2\pi}\int_\Omega \frac{\partial^2 \Phi_\Omega(\varepsilon_N)}{\partial \varepsilon_N \partial \varepsilon_N}N_i N_j N_s N_t d\Omega + \frac{\partial^2 \Psi(\varepsilon_V)}{\partial \varepsilon_V \partial \varepsilon_V}\delta_{ij}\delta_{st} \tag{21}$$

In particular, when the energy functions

$$\Phi_\Omega(\varepsilon_N) = \frac{1}{2}\varepsilon_N E_N \varepsilon_N, \qquad \Psi(\varepsilon_V) = \frac{1}{2}\varepsilon_V E_V \varepsilon_V \tag{22a,b}$$

where E_N and E_V are the elastic constants, respectively, the constitutive equations reduce to the ones of an isotropic linear elastic solid. By substituting Eqs. (22ab) into Eq. (21) and making use of the relation

$$\int_\Omega N_i N_j N_s N_t d\Omega = \frac{2\pi}{15}(\delta_{ij}\delta_{st} + \delta_{is}\delta_{jt} + \delta_{it}\delta_{js}) \tag{23}$$

it can be directly verified that

$$C_{ijst} = E_N(\delta_{ij}\delta_{st} + \delta_{is}\delta_{jt} + \delta_{it}\delta_{js}) + E_V\delta_{ij}\delta_{st} \tag{24}$$

By comparing Eq. (24) with the standard isotropic linear elastic constitutive equation

$$C_{ijst} = \lambda\delta_{ij}\delta_{st} + \mu(\delta_{is}\delta_{jt} + \delta_{it}\delta_{js}) \tag{25}$$

the elastic constants E_N and E_V can be identified in terms of the Lamé constants λ and μ,

$$E_N = \mu, \qquad E_V = \lambda - \mu \tag{26a,b}$$

Eqs. (18-21) define a continuum constitutive model for non-dissipative materials, called the orientation element based constitutive model (OEBCM) in this paper. It is known that from the atomistic viewpoint

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the contribution of the two-body potential to the free energy often plays a more important role than the embedding energy of atoms. Eq. (26ab) also show that the elastic constant E_V completely disappears when Poisson's ratio of engineering materials is 1/4. Therefore, we will first discuss the numerical implementation of the OEBCM without the contribution of the embedding energy in the next section.

LATTICE MODEL

Usually, the OEBCM is numerically implemented in the context of the finite element method, and the constitutive law of materials characterized by Eqs. (18-21) is evaluated at each quadrature points of a set of finite elements. Meanwhile, the truss lattice model, which is directly derived from the discretization of the OEBCM, offers an attractive alternative way of the numerical implementation of the OEBCM.

Subdivide the hemispherical envelop into M discrete contiguous solid angles, $\Delta\Omega^{(m)}$, each associated with a corresponding discrete orientation $N_i^{(m)}$. These solid angles do not overlap and collectively they span the hemisphere exactly and completely. The total energy of the infinitesimal neighborhood of the material particle can then be approximated by

$$E(\varepsilon) = \frac{15V}{2\pi} \int_\Omega \Phi_\Omega(\varepsilon_N) d\Omega \approx \sum_{m=1}^{M} E^{(m)} = \frac{15V}{2\pi} \sum_{m=1}^{M} \Phi^{(m)}(\varepsilon_N^{(m)}) \Delta\Omega^{(m)} \tag{27}$$

On the other hand, select a 1D truss element with orientation $N_i^{(m)}$, length $l^{(m)}$, and let its energy

$$\hat{E}^{(m)} = \hat{\Phi}^{(m)}(\varepsilon_N^{(m)} l^{(m)}) \tag{28}$$

From Eqs. (27) and (28), when the energy of the truss element with orientation $N_i^{(m)}$

$$\hat{\Phi}^{(m)}(\varepsilon_N^{(m)} l^{(m)}) = \frac{15V}{2\pi} \Phi^{(m)}(\varepsilon_N^{(m)}) \Delta\Omega^{(m)} \tag{29}$$

The infinitesimal neighborhood of the material particle can be replaced with an energy equivalent lattice cell with M truss elements oriented M directions. The unit cell with the compatible deformation with ε, is greatly much coarser than the true atomic one, but can approximately performs the mechanical behavior of the assemble of atoms with the enormously large number of degrees of freedom.

In particular, for a linear elasticity solid with the free energy

$$\Phi^{(m)}(\varepsilon_N^{(m)}) = \frac{1}{2} \varepsilon_N^{(m)} E_N^{(m)} \varepsilon_N^{(m)} \tag{30}$$

where $E_N^{(m)}$ is a elastic constant, the energy of the truss element with orientation $N_i^{(m)}$ and its the elastic stiffness $k^{(m)}$ have the format, respectively

$$\hat{\Phi}^{(m)}(\varepsilon_N^{(m)} l^{(m)}) = \frac{1}{2} k^{(m)}(\varepsilon_N^{(m)} l^{(m)})^2, \qquad k^{(m)} = \frac{15V E_N^{(m)} \Delta\Omega^{(m)}}{2\pi(l^{(m)})^2} \tag{31}$$
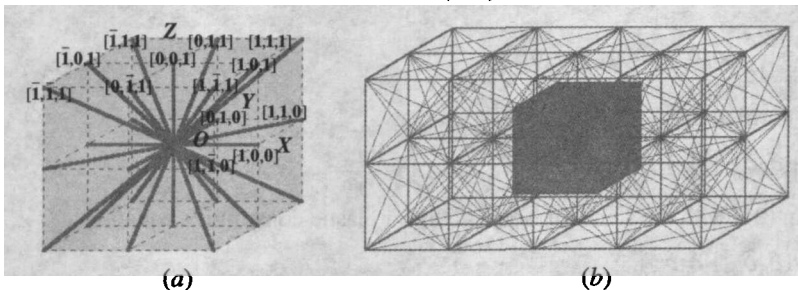

Fig. 1 (a) Three-dimensional regular lattice unit cell, (b) The periodic lattices made up of the unit cell

Fig. 1(a) shows a cubic lattice cell with 13 truss elements oriented in {1,0,0}+{1,1,0}+{1,1,1} directions. Taking this three-dimensional lattice cell as the unit cell of a periodic discrete lattice shown in Fig. 1(b) [9]. The constructed truss lattice model can be conceived as an alternative way of the numerical

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implementation of the OEBCM, instead of the finite element method. Additionally, when the contribution of the embedding energy of atoms to the free energy is considered, its effect can be incorporated into the lattice model as the body force.

TRUSS-TYPE LATTICE STRUCTURED MATERIALS

Materials with lattice-like structures at length scales ranging from millimetres to tens of centimeters have been widely investigated in recent years [7]. Obviously, materials with lattice-like structures can be effectively modeled as the truss lattice model. An infinite periodic latticed structure composed of truss elements can further be equivalent to a continuum body modeling by the OEBCM. Therefore, the optimum design of as well as the investigation of the effective mechanical properties of the truss-type lattice structured materials can also be cased into the framework of the discretization of the OEBCM.

CONCLUSIONS

1) Within the framework of the embedded-atom method with the CBR, we formulate the Helmholtz free energy used in thermodynamics, and then construct the OEBCM for non-dissipative materials.
2) By introducing the internal state variables into the Helmholtz free energy, the OEBCM seems to be highly promising for the solution of engineering problems involving plasticity and damage process with a greatly simplified mathematical description.
3) The discretization of the integration furnishes a unified framework for the development of the truss lattice models and the truss-type lattice structured materials.

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