C. R. Mecanique 342 (2014) 315–325

Contents lists available at ScienceDirect

Comptes Rendus Mecanique

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Frontiers of micro and nanomechanics of materials: Soft or amorphous matter, surface effects

Determinations of both length scale and surface elastic parameters for fcc metals

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ARTICLE INFO

Article history:
Received 29 April 2013
Accepted 21 October 2013
Available online 24 April 2014

Keywords:
Trans-scale mechanics
Cauchy–Born rule
Surface energy density
Length scale
Surface elastic parameter

ABSTRACT

In the present research, a systematical study of trans-scale mechanics theory is performed. The surface/interface energy density varying with material deformation is considered, and the general surface/interface elastic constitutive equations are derived. New methods to determine the material length scale parameter and the surface elastic parameters based on a simple quasi-continuum method, i.e. the Cauchy–Born rule, are developed and applied to typical fcc metals. In the present research, the material length parameters will be determined through an equivalent condition of the strain energy density calculated by adopting the strain gradient theory and by adopting the Cauchy–Born rule, respectively. Based on the surface constitutive equations obtained in the present research, the surface elastic parameters are calculated by using the Gibbs definition of surface energy density and the Cauchy–Born rule method.

1. Introduction

Differing from conventional material, modern material in overall or in local is precisely designed and manufactured starting from its microstructure. This is a major feature for modern material. Therefore, modern materials often display good mechanical properties. It is expectable that with wide applications of modern materials, quality and life of products should be improved greatly. However, mechanical behavior of modern materials is microstructure sensitive, and generally speaking conventional mechanics theories cannot characterize the mechanical behavior of modern materials effectively, so that an effective mechanics theory is needed, which can describe the above-mentioned trans-scale mechanics behavior.

Previously, one investigated the above problems mainly from two independent ways: one of them was to present the strain gradient theories for describing the strain gradient effects caused by the material microstructure formation and evolution; the other one was to develop the surface/interface theories for describing the surface/interface effects due to nanostructure deformation and evolution around the surface or interface.

It is well known that there exist many researches on both strain gradient theories and surface/interface effects. In the present introduction, we intend to give a brief review of the types of size-effect study methods, and gradually introduce the trans-scale mechanics theory and the parameter identification problem, instead of providing with mass literatures.

Size effect of the mechanical behavior of microstructured material can be interpreted effectively by adopting strain gradient theories, in which through considering the contributions of the higher-order stresses and strain gradients, the material-inherent scales are introduced and the size effect of mechanical behavior of microstructured materials can be

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http://dx.doi.org/10.1016/j.crme.2014.03.004
1631-0721/

characterized [1]. Until now, the research work on the strain gradient theories has been performing [1–6]. Previously, the length scale parameters included in the strain gradient theories were measured mainly through simulating experimental results of small-size specimens [7,8]. Some investigators studied the mechanical behavior size effect for microstructured materials by considering micro-polar effect [9]. When material cell size is at the nanometer scale, since the specific surface area (SSA) is so high to reach the order of $(10^6–10^9)/\mathrm{m}$ [10], the magnitude of surface/interface energy is high to be comparable to that of the strain energy, and surface/interface theories considering the surface/interface effects were presented for describing the size effect of the mechanical behavior [10–13]. However, the size effects characterized by the surface/interface theories happen only within a very small scale (below 10 nanometers). Until now, the research work on the surface/interface effects has been performing [14–20].

Summarizing previous researches on the size effects, only considering the strain gradient effect the mechanical behavior of nanostructured materials, cannot be described effectively, while merely considering the surface/interface effect the mechanical behavior of microstructured materials is not described well. Therefore, we presented a trans-scale mechanics theory by which both strain gradient effect and the surface/interface effect are considered simultaneously, and we built up an overall frame of the theory and made the theory applied to the analysis of grain size effect of the nanocrystalline materials [21]. In a previous version of trans-scale mechanics theory, the surface/interface energy density was taken as a material parameter unchanged with deformation.

From materials physics, the surface/interface effect is the state difference between atoms situated at the surface/interface and those located within the material's interior. Different states of atoms bring different energies, depending on atom location—on the surface/interface or at the material interior—, which influences the overall mechanical behavior of materials. In studying the surface/interface effect, a most fundamental concept is the surface/interface free energy. There have been many researches on the surface/interface energy. A definition of surface energy was presented by Gibbs [22]. Surface energy describes the surplus energy of surface atoms relative to the interior atoms. Currently, there are three kinds of approaches for determining surface energy, which are experimental measurement, theoretical modeling, and numerical simulation [23]. Surface stress is also an important quantity to describe the solid surface behavior [22]. Differing from liquid surface, solid surface will cause the surface stress. Shuttleworth defined the surface stress as a differential of surface energy to surface strain [24]. Surface stress has a considerable influence on the nanostructured material behavior [25].

There have been many researches on the surface stress and surface constitutive relation. Maede and Vanderbilt [26] and Needs [27] studied the surface stresses of semiconductor element and metal element by using *ab initio* calculations. Shenoy [28] studied the surface constitutive relation and derived the surface elastic constants, and he obtained the formulas of the surface elastic parameters. Mi et al. [29] and Pahlevani and Shodja [30] investigated the surface stress and the surface elastic parameters through molecular dynamics (MD) simulation.

In the present research, a systematical study on the trans-scale mechanics theory is performed. The surface/interface energy density varying with the material's deformation is considered, and general surface/interface elastic constitutive equations are derived. New methods for determining the material length scale parameter and the surface elastic parameters based on a simple quasi-continuum method, the Cauchy–Born rule (CBR), are developed and applied to typical fcc metals.

Determination of material length parameters is different from conventional methods that simulate experimental results of small-size specimens. In the present research, the material's length parameters will be determined through an equivalent condition of the strain energy density calculated by adopting the strain gradient theory and by adopting the CBR, respectively.

In the determination method of surface elastic parameters, firstly, based on the surface constitutive equations obtained in the present research, the relations of surface elastic parameters with surface energy density are derived; secondly, surface elastic parameters are calculated by using Gibbs' definition of surface energy density and the CBR method.

2. Trans-scale mechanics theory

2.1. Variation equations of the total potential for solids

In conventional theory, the total potential for solids is:

$$\int_V \boldsymbol{\sigma}\delta\boldsymbol{\varepsilon}\,\mathrm{d}V - \int_V \bar{\mathbf{f}}\delta\mathbf{u}\,\mathrm{d}V - \int_S \bar{\mathbf{t}}\delta\mathbf{u}\,\mathrm{d}S = 0 \tag{1}$$

where $(\boldsymbol{\sigma}, \boldsymbol{\varepsilon}, \mathbf{u}, \bar{\mathbf{t}}, \bar{\mathbf{f}})$ are the tensor or vector of stress, strain, displacement, traction and volume force.

For trans-scale mechanics theory, considering both strain gradient effect and surface/interface effect, the variation equation of the total potential can be expressed as follows [21]:

$$\int_V (\boldsymbol{\sigma}\delta\boldsymbol{\varepsilon} + \boldsymbol{\tau}\delta\boldsymbol{\eta})\,\mathrm{d}V + \delta\int_{S'} \gamma\,\mathrm{d}S' - \int_V \bar{\mathbf{f}}\delta\mathbf{u}\,\mathrm{d}V - \int_S \left(\bar{\mathbf{t}}\delta\mathbf{u} + \bar{\mathbf{S}}_0{}^s\delta\boldsymbol{\varepsilon}^s + \bar{\mathbf{r}}\cdot(\delta\mathbf{u}\mathbf{n}\cdot\nabla)\right)\mathrm{d}S = 0 \tag{2}$$

where $\boldsymbol{\tau}$ and $\boldsymbol{\eta}$ are the tensors of higher-order stress and strain gradient, $\boldsymbol{\tau}\delta\boldsymbol{\eta}$ is the variation of strain energy density contributed from strain gradient effect, $\bar{\mathbf{r}}\cdot(\delta\mathbf{u}\mathbf{n}\cdot\nabla)$ is the surface-specific work done by higher-order stress moment, γ is