Available online at www.sciencedirect.com

SciVerse ScienceDirect

Acta Materialia 61 (2013) 89–102

Acta MATERIALIA

www.elsevier.com/locate/actamat

# Concurrent atomistic and continuum simulation of strontium titanate

Shengfeng Yang, Liming Xiong, Qian Deng, Youping Chen *

*Department of Mechanical and Aerospace Engineering, University of Florida, Gainesville, FL 32611, USA*

Received 4 July 2012; received in revised form 30 August 2012; accepted 10 September 2012
Available online 26 October 2012

**Abstract**

This paper presents a concurrent atomistic–continuum methodology (CAC) to simulate the dynamic processes of dislocation nucleation and migration as well as crack initiation and propagation in complex crystals. The accuracy and efficiency of the method is tested with respect to the molecular dynamics (MD) method through simulations of the dynamic fracture processes in strontium titanate under a combination of tension and shear loading and the dislocation behavior under nanoindentation. CAC simulation results demonstrated a smooth passage of cracks and dislocations through the atomistic–continuum interface without the need for additional constitutive rules or special numerical treatment. Although some accuracy is lost in CAC simulations as a consequence of a 98.4% reduction in the degrees of freedom, all the CAC results are qualitatively and quantitatively comparable with MD results. The stacking fault width and nanoindentation hardness measured in the CAC simulations agrees well with existing experimental data. Criteria for cleavage and slip in ionic materials are verified. The need to include the internal degrees of freedom of atoms in concurrent atomistic–continuum methods for polyatomic crystalline materials is confirmed.


*Keywords:* Concurrent atomistic–continuum simulation; Dislocation; Dynamic fracture; Strontium titanate

## 1. Introduction

In the last two decades, a large body of literature in science and engineering has focused on various methods of fitting together simulation models of two or more scales, with the hope to expand the atomistic simulation-based predictive capability from nanometer to micron or larger length scales, leading to the development of various multiscale models. Despite intense research efforts, however, attempts to develop a general multiscale methodology have not succeeded. In addition to non-equilibrium and finite-temperature phenomena, dynamic behavior of polyatomic materials, i.e., materials that have more than one atom in the primitive unit cell, has been a significant challenge to coarse-grained (CG) atomistic or concurrently coupled atomistic–continuum methods.

The classical methods for coarse-graining monatomic crystals to find the elastic constants are the method of long waves and the method of homogeneous deformations (the Cauchy–Born hypothesis) [1–3]. For polyatomic crystals, the existence of inner displacements or internal strains increases the mathematical complexity of the formulation of the methods. As a consequence, most existing coupled or mixed atomistic–continuum methods that use atomistic dynamics at the nanoscale and classical elasticity at the mesoscale were formulated for monatomic crystals and are not applicable to polyatomic or multi-atomic crystalline solids.

One currently popular multiscale method is the quasicontinuum method (QC). QC was originally formulated for simple Bravais crystals based on the energy-minimization technique, with the aim of reproducing the results of standard lattice statics at a fraction of the computational cost [4]. An attempt to extend the QC method to simulate materials with multiple atoms in a unit cell was made in 1999 [5]. In the modified QC formulation, the strain energy

* Corresponding author. Tel.: +1 352 392 8494.
*E-mail address:* ypchen2@ufl.edu (Y. Chen).

1359-6454/$36.00 
http://dx.doi.org/10.1016/j.actamat.2012.09.032

is expressed as a function of the deformation gradient $\mathbf{F}$ and inner displacements $\xi^n$, where $n = 1, \ldots, N_a$, with $N_a + 1$ being the number of the basis atoms per Bravais site. For a given macroscopic deformation, the strain energy is minimized with respect to the inner displacements, i.e.,

$$\left.\frac{\partial W}{\partial \xi^n}\right|_{\mathbf{F}} = 0, \quad n = 1, \ldots, N_a \tag{1}$$

After minimization, the equilibrium inner displacements $\hat{\xi}^n = \hat{\xi}^n(\mathbf{F})$ are obtained, which implies that the strain energy is only a function of the deformation gradient:

$$W = W(\mathbf{F}, \hat{\xi}^n) = W(\mathbf{F}, \hat{\xi}^n(\mathbf{F})) \equiv W(\mathbf{F}) \tag{2}$$

This modified QC formulation was applied to simulate silicon nanoindentation [6]. In the course of the simulation, some of the finite elements (FE) became unstable, and the relative positions of the basis atoms changed by a large amount. To identify the new phase, the deformation gradient and the positions of the basis atoms in the FE were used to create an infinite silicon crystal, and an additional fully resolved atomistic simulation was then performed. Separated from the QC simulation, this atomistic model of crystal was relaxed to its local minimum energy well, in order to identify the phase associated with the QC FE model.

The modified QC method attempts to extend the method of static simulations of monatomic lattice to general crystalline materials, but, for simulations of phase transformation, an additional atomistic simulation is required. Another common feature in all QC models is that discontinuities such as cracks or dislocations cannot pass from the atomic region to the CG region. It was shown in a recent simulation by the monatomic QC with adaptive mesh that, in order to accommodate dislocations, the coarse mesh in QC models needs to be adaptively refined down to the atomic scale to capture dislocation nucleation and allow migration. A recent simulation result shows that nearly a fully atomistic resolution is required in the entire model for simulations involving dislocations [7].

For passing defects from the atomic to the CG region, CADD has been the most successful multiscale method for monatomic crystalline materials. CADD combines the atomistic methods and continuum defect methods in one computational scheme [8]. It allows dislocations nucleated in the atomistic region to pass into the continuum region through algorithms of detecting dislocations near the atomic/continuum interfaces and moving dislocations across the interfaces. The method was well demonstrated through simulations of twining in face centered cubic metals [9]. A key issue with CADD is that the passing methodology in CADD restricts its applications to two-dimensional problems, and so extension of CADD to thee-dimensional (3-D) or curved dislocations is difficult. Another domain decomposition-based multiscale model is the combination of the extended finite element method (XFEM) and the bridging domain method (BDM) in one computer model [10]. This method allows the discontinuities from the atomistic region to pass into the continuum region through the enrichment of the FEM with a Heaviside step function. The compatibility of the atomistic and continua domains is enforced by a Lagrange multiplier field. In this XFEM + BDM method, additional rules are needed to detect dislocations and also to coarse-grain the domain vacated by dislocations. In addition to 3-D and curved dislocations, determination of equivalent continuum descriptions of discontinuities from atomistic displacements is very challenging. Moreover, the description of the continuum region is only valid for monatomic lattice.

The objective of this paper is to demonstrate a new concurrent atomistic–continuum (CAC) methodology to simulate the dynamic process of dislocation nucleation and migration as well as crack initiation and propagation in materials with complex crystal structures. The CAC method is based on a unified atomistic–continuum formulation for general crystals [11–14] and a modified FEM for modeling of discontinuous material behavior [15]. It removes the majority of degrees of freedom in the CG domain and allows nucleation and propagation of dislocations and cracks in either the atomistic or the continuum domain as consequences of the governing equations, without the need for additional constitutive rules or special numerical treatments for discontinuities. It also allows the defects to pass from the atomistic to the continuum domain and vice versa [16–19]. The only constitutive law for both the atomistic and the continuum domains is the force field, and both the atomistic and continuum domains are governed by the same set of balance equations.

The perovskite oxides strontium titanate $SrTiO_3$ (STO) were chosen in this work because perovskite oxides in general have a broad application, and STO in particular is one of the most commonly used substrates and also a potential thermoelectric material [20]. The study of their mechanical properties is very important, since they can influence the functionality [21,22]. To date, however, limited atomic-level calculations have been performed to study experimentally observed phenomena in STO, such as brittle fracture during tension and plastic behavior during nanoindentation [23]. Recently, Hirel et al. [24] conducted a molecular dynamics (MD) simulation of STO to investigate its plastic behavior. By introducing dislocations before relaxation, the dissociation distances of edge and screw dislocations are predicted and compared with experiments. Owing to the limitation of length and time scales of MD simulations, the simulation is restricted to small models with one or two dislocations and thus neglects the long-range interaction between dislocations. The highly complex structure of the dislocation core and long-range interaction between dislocations make the slip process of dislocation a typical multiscale phenomenon, which requires modeling in various scales.

The paper is organized as follows. The CAC methodology is briefly introduced in Section 2; the computer models