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Ab initio calculations of mechanical properties: Methods and applications

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ABSTRACT

This article attempts to critically review a rather extended field of ab initio calculations of mechanical properties of materials. After a brief description of the density functional theory and other approximations utilized in a majority of ab initio calculations, methods for predictions of elastic constants and moduli are presented. A relatively large space is devoted to computations of theoretical strength under various loading conditions. First we focus on results for perfect crystals and make an overview of advanced approaches to crystal stability. As case studies, elastic stability conditions defined according to both the adopted definition of elastic coefficients and the kind of applied loading are shown for isotropic tensile loading of molybdenum crystal and a model of microscopic deformation is illustrated for a soft phonon found in the dynamic stability analysis of isotropic loading of platinum crystal. Collected values of ideal strength under uniaxial/isotropic tension and simple shear for selected metallic and covalent crystals are discussed in terms of their comparison with available experimental data. Further attention is paid to results of studies on interfaces and grain boundaries. Applications of computed values of the moduli and the theoretical strength to prediction of intrinsic hardness and brittle/ductile behavior of crystalline materials and simulation of pop-in effect in nanoindentation tests are also included. Finally,

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remarks about possible topics for future ab initio studies and challenges for further development of computational methods are attached.

Contents

1. Introduction

The objective of most ab initio (or first-principles) approaches based on fundamental quantum theory is to calculate stationary states of electrons in the electrostatic field of atomic nuclei, i.e., the electronic structure. The energy of this ground state can then serve as a basis for investigation of displacements of the nuclei which leads to determination of many macroscopic properties important in technology. First attempts to develop applicable theories were made in the late 1920s, a few years after the derivation of the Schrödinger equation. However, a really successful approach providing a solution of this equation for many-body problem that is relevant to solids was done almost 50 years later. The density functional theory (DFT) was invented to include correlation effects without using the very costly wavefunction methods. Nowadays, most ab initio methods used in materials science and solid state physics are based on the DFT.

The main advantage of ab initio approach is its independence on experimental data. Unlike in the case of semi-empirical methods, there is no need for calibration or fitting parameters. Thus, ab initio methods can also be used for calculations of some structural and mechanical characteristics of hypothetical systems, i.e., for prediction of properties of materials that have not yet been developed. This is, however, not the main aim of this article. Here we focus rather on the studies on materials behavior under large deformations far from the equilibrium state. Such investigations can provide a better understanding of micromechanisms of materials failure. This article may be considered, on one hand, as an up-date and continuation of an earlier review [1] devoted solely