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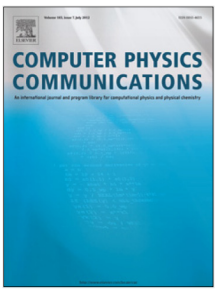

Ab initio calculations of pressure-dependence of high-order elastic constants using finite deformations approach

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Abstract

We present a description of a technique for *ab initio* calculations of the pressure dependence of second- and third-order elastic constants. The technique is based on an evaluation of the corresponding Lagrangian stress tensor derivative of the total energy assuming finite size of the deformations. Important details and parameters of the calculations are highlighted. Considering body-centered cubic Mo as a model system, we demonstrate that the technique is highly customizable and can be used to investigate non-linear elastic properties under high-pressure conditions.

Keywords: ab initio calculations, elastic moduli, pressure effects in solids and liquids
PACS: 31.15.A-, 62.20.de, 62.50.-p

1. Introduction

There is a notable increasing interest in higher order elastic constants (HOEC) of solids [1, 2, 3, 4, 5, 6]. The study of nonlinear elasticity helps to reveal the details of complex behavior of materials. For example, investigating the trends of HOECs one can understand mechanisms of structural instabilities [3] or incorporate proper description of nonlinear elasticity in case where there is a discrepancy between more general theory and experiment [4].

Usually the elasticity theory is considered in an approximation of infinitesimal deformations [7]. Such approach is the most logical choice, when the applied deformation is small compared to inter-atomic distances of undeformed material. But inter-atomic potentials in real materials are anharmonic. The explicit accounting of anharmonicity in study of solids becomes more and more prominent. This is quite evident when theoretical investigation of materials is performed for realistic conditions including the extreme ones, which are, for instance, of interest for cutting edge studies [8, 9]. Standard theoretical methods

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