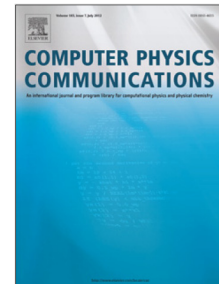


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Ab initio calculations of pressure-dependence of high-order elastic constants using finite deformations approach

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20
21 **Abstract**

22 We present a description of a technique for *ab initio* calculations of the pressure
23 dependence of second- and third-order elastic constants. The technique is based
24 on an evaluation of the corresponding Lagrangian stress tensor derivative of
25 the total energy assuming finite size of the deformations. Important details and
26 parameters of the calculations are highlighted. Considering body-centered cubic
27 Mo as a model system, we demonstrate that the technique is highly customizable
28 and can be used to investigate non-linear elastic properties under high-pressure
29 conditions.
30

31 *Keywords:* ab initio calculations, elastic moduli, pressure effects in solids and
32 liquids

33 *PACS:* 31.15.A-, 62.20.de, 62.50.-p
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37 **1. Introduction**

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

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