

Phonon dispersion curves of transition metals using modified general tensor force model

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Abstract. The general tensor force model has been modified by incorporating separately the electron-ion interactions. The model satisfies the translational symmetry requirements of the lattice and is used to obtain the phonon dispersion curves of chromium, molybdenum and tungsten. The agreement between the theoretical and experimental frequencies is very good.

Keywords. Umklapp processes; dispersion curves; transition metals; interference factor; tensor force.

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1. Introduction

The general tensor force model (Begbie and Born 1947) which assumes the atomic interactions to be two-body interactions but imposes no restriction on the nature of such interactions has so far been used, with large number of force constants, mainly to analyze the experimental dispersion curves of solids. However, recently Ramamurthy and Satish Kumar (1985) used this model by incorporating volume forces separately to study the lattice dynamics of alkali metals and obtained excellent results for all alkali metals including the cross-over of lithium branches along $[\zeta 00]$ direction, without violating the translational symmetry requirements of the lattice. Inspired by the success of the model we have attempted to extend it to the study of transition metals with bcc structure. Our motivation for such studies is from the fact that these metals are more complicated as their conduction electrons are relatively less free and their number per unit volume is not fixed as they lie in the (Spd) hybrid states. Large values of their elastic constants indicate strong electron-ion interactions having considerable influence over the computed phonons and therefore these metals will provide a rigorous test for this model. This paper, therefore, deals with the study of chromium, molybdenum and tungsten belonging to VIB group. Such studies for the VB group will be reported later.

2. Theory

To obtain the phonon frequencies, the ion-ion interactions are expressed in terms of tensor forces (Begbie and Born 1947) and the electron-ion interactions in terms of the volume forces which satisfy the translational symmetry requirements of the lattice. Restricting the range of ion-ion interactions upto the third nearest neighbour