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Abstract—Nonlinear atomic vibrations in a model of long-period stacking ordered (LPSO) structure in magnesium is investigated numerically. We search nonlinear vibrations in the gap of the dispersion relation by using of the coupled numerical method of molecular dynamic (MD) simulation and the Newton-Raphson method. We also discuss the dynamics of atoms after the nonlinear vibration becomes unstable.

1. Introduction

Recently, synchronized long period stacking ordered (LPSO) structure has been studied extensively as to their uniquely mechanical characteristics. Synchronized LPSO appears in magnesium alloys with rare earth element as a layered structure in which modulation of condensation of rare earth element and structure of stacking fault are synchronized. From the viewpoint of dynamics of atoms, vibration in the LPSO structure is interesting problem since the LPSO structure has two substructures with different scales, that is, atomic distance and length of modulation or stacking fault. This structural specification leads special vibrational property even in linear vibration. Moreover, vibration of finite amplitude is important. Therefore it is expected that more complex behavior occur due to both LPSO structure and nonlinearity of interaction between atoms. In this study, we investigate nonlinear vibration of the LPSO structure numerically.

2. Models

We consider the three dimensional atomic model. Hexagonal close-packed structure of magnesium atoms is formed. Embedded atom method potential proposed by Liu is used for describing the interaction between magnesium atoms. Modulation of the concentration of other atom is modeled by changing mass of the some layers of atom.

3. Numerical Calculation

We search the nonlinear vibration mode that corresponds to linear phonon mode. The nonlinear vibration mode is calculated by Newton-Raphson method in which initial guess solution is phonon mode. The linear phonon mode is calculated by solving the eigenvalue problem of dynamical matrix determined by the structure of crystal and interaction. Fig. 1 shows the dispersion relation of the phonon modes of layered structure with period two along to z-axis.

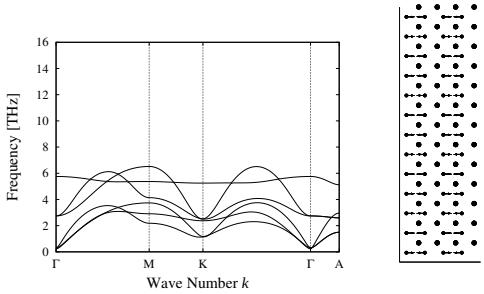

Figure 1: Phonon mode layered structure with period 2. (Left) dispersion relation, (Right) displacement of atoms of the highest frequency mode.

Fig. 2 shows the relation between frequency and amplitude of nonlinear vibrations. We can see the increase of the frequency due to the nonlinearity of the interaction.

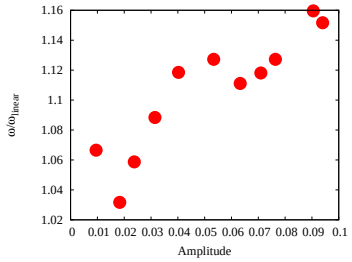

Figure 2: Relation between amplitude and frequency of nonlinear vibration mode that corresponds to the phonon mode with highest frequency.

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