Two-dimensional discrete breathers in hcp titanium

O V Bachurina1, R T Murzaev2, M N Semenova3, A S Semenov3, D S Ryabov4, G M Chechin4, E A Korznikova2 and S V Dmitriev2,5

1 Ufa State Petroleum Technological University, Ufa 450062, Russia
2 Institute for Metals Superplasticity Problems, Ufa 450001, Russia
3 North-Eastern Federal University n.a. M.K. Ammosov, Polytechnic Institute (branch) in Mirny, Mirny 678170, Sakha (Yakutia), Russia
4 Southern Federal University, Rostov-on-Don 344006, Russia
5 National Research Tomsk State University, Tomsk 634050, Russia

E-mail: dmitriev.sergey.v@gmail.com

Abstract. Recently delocalized nonlinear vibrational modes (DNVMs) have been derived for a two-dimensional (2D) triangular lattice and their frequencies as the functions of amplitude have been calculated for a 2D Morse crystal. A 3D hcp lattice is formed by certain stacking of 2D triangular lattices. In the present work, we attempt to excite eight DNVMs with in-plane atomic displacements in a single plane of hcp titanium, modelled using many-body interatomic potentials. It is found that three of eight DNVMs produce long-lived 2D discrete breathers (DBs) in a titanium crystal. A 2D DB is delocalized in two spatial dimensions and localized in the third one, so that atoms of only one atomic plane have large vibrational amplitudes. The frequencies of the newly found DBs lie above the small-amplitude phonon spectrum of titanium and grow with increasing amplitude. Thus, we report on three novel 2D DBs in hcp metal. Our results open the route to finding new types of DBs in pure metals.

1. Introduction

Discrete breathers (DBs) are spatially-localized, large-amplitude vibrational modes in discrete nonlinear lattices [1-3]. DBs have frequencies outside the spectrum of small-amplitude lattice vibrations. Their frequency, for sufficiently large amplitudes, can leave the spectrum due to the nonlinearity of the lattice, since the frequency of the nonlinear vibrational mode depends on its amplitude. For the soft (hard) type of nonlinearity, DB frequency decreases (increases) with its amplitude. The existence of DBs in crystal lattices has been proved by a number of molecular dynamics studies [2-18], and recently in several works using the ab initio approach in frames of the density functional theory [19,20]. Experimental observation of DBs in crystals is a challenge due to their atomic-scale size and the lifetime from 10 to 1000 atomic vibrations. Nevertheless, their successful identification has been summarized in the recent review [2]. Until 2011, it was believed that pure metals could not support DBs because interatomic interactions were soft, and, in this situation, only crystals having a gap in the phonon spectrum could support DBs [16]. However, Haas et al. demonstrated the existence of DBs in fcc Ni and bcc Nb [11]. Later it was shown that interatomic interactions were actually soft at large distances and hard at small distances [18]. When the hard core of the interatomic potential makes a greater contribution to the dynamics of nonlinear excitation than...
its soft tail, the frequency of excitation can grow with amplitude and cross the upper edge of the phonon spectrum. DBs in pure metals were analyzed in the works [12-14].

Recently it was realized that 2D crystals could support 1D DBs (delocalized in one dimension and localized in another), while in 3D crystals both 1D and 2D DBs were possible. In particular, a 1D DB has been analyzed in fcc aluminum with large-amplitude oscillations of atoms in a single close-packed atomic row [15]. In the present study, we discuss 2D DBs in hcp titanium, simulated using molecular dynamics. The considered nonlinear, large amplitude oscillations are localized in a single basal atomic plane of the crystal. The amplitudes of atomic vibrations decay exponentially with a deviation from the plane, where a 2D DB is excited.

The main problem in excitation of a DB in molecular dynamics simulations is to find the proper initial conditions. It has been proved that delocalized nonlinear vibrational modes (DNVMs), also called one-dimensional bushes of nonlinear normal modes, can be very helpful in solving this problem [5,18]. DNVMs are the exact solutions to the nonlinear equations of atomic motion, regardless the interatomic potentials used in simulations, because DNVMs are dictated by the lattice symmetry and are found with the use of the group theory [21]. Note that the basal plane of the hcp crystal is a 2D triangular lattice, for which Chechin and Ryabov derived eight DNVMs with in-plane atomic displacements [22]. We excite these modes in a single basal plane of titanium and analyze the lifetime of such excitations. If the lifetime is long, the obtained excitation is called a 2D DB.

2. Simulation details

We consider hcp titanium modeled with the use of many-body interatomic potentials obtained with the help of the embedded-atom method (EAM) [23]. The computational cell includes 20 basal planes with 12\times12 atoms in each plane. The lattice parameters of titanium are $a=2.951 \text{ Å}, c=4.684 \text{ Å}$. Periodic boundary conditions are used. Thermal fluctuations are not introduced in the system.

The initial conditions are set by applying an initial shift to the atoms in single basal plane according to the pattern of one of the eight DNVMs with in-plane atomic displacements derived by Chechin and Ryabov [22]. Three of the eight DNVMs are shown in figure 1a, the other modes can be found in [22]. The length of the arrows is equal to $D_0$, which defines the initial amplitude of the DNVM. The
initial atomic displacements in all other basal planes are equal to zero, and the initial velocities of all atoms in the computational cell are equal to zero. In the work [22], the frequency as a function of amplitude was calculated for all eight DNVMs excited in a 2D Morse crystal. This result is shown in figure 1 b. It can be seen that in the studied range of $D_0$, only DNVMs 2, 3, 5 and 7 have frequencies above the upper edge of the phonon spectrum, which is indicated by the horizontal dashed line.

3. Numerical results and discussion

In our simulations, all eight DNVMs with in-plane displacements derived for a triangular lattice have been analysed. Only three of them have produced long-lived 2D DBs. These are DNVMs 2, 5 and 7 shown in figure 1 a. It is not surprising that DNVMs 1, 4, 6, and 8 did not produce a long-lived vibrational mode, because in a 2D Morse lattice they have frequencies within the phonon band. DNVM 3 has a frequency above the phonon band in a 2D Morse lattice only for sufficiently large vibrational amplitude. It should be pointed out that when a DNVM is excited in a 2D triangular lattice, it does not interact with other vibrational modes and it keeps its energy constantly in time. On the other hand, when a DNVM is excited in a single basal plane of the hcp lattice, a part of its energy is given to the neighbouring atomic planes, and this is the reason for the decay of DNVM 3, which has a frequency above the phonon spectrum of the 2D Morse lattice only for sufficiently large amplitude.

In figure 2 (d), the total (kinetic plus potential) energy per atom in a single basal plane is plotted for DNVMs 2, 5 and 7 as a function of the initial displacements of atoms, $D_0$. It can be seen that the maximal energy per atom is approximately equal to 0.5 eV and the maximal initial displacement is about 0.5 Å. For larger initial displacements, strong energy radiation from the excited basal plane is observed.

4. Conclusions

For the first time, three new 2D DBs were obtained and analysed in an hcp crystal using titanium as an example. Large amplitude vibrations in the described 2D DBs take place in a single basal plane. The patterns of atomic vibrations in this plane correspond to DNVMs 2, 5, and 7 described in [22]. It would be interesting to analyze the possibility of the existence of similar 2D DBs in fcc pure metals.
Acknowledgements
The work of A.S.S. (discussion of the numerical results) was supported by the Russian Foundation for Basic Research, grant no. 18-32-00171_mol_a. D.S.R and G.M.Ch. have worked under state assignment no. 3.5710.2017/8.9 (derivation of DNVM and discussion of the results). E.A.K. thanks the Russian Foundation for Basic Research, grant no. 17-02-00984_a (writing the paper). S.V.D. thanks the Russian Science Foundation, grant no. 16-12-10175, for their financial support (design of the research). This work was partly supported by the state assignment of IMSP RAS.

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