

Surface discrete breathers in Pt₃Al

Elena A. Korznikova^A, Pavel V. Zakharov^B and Sergey V. Dmitriev^{A,C}

^AInstitute for Metals Superplasticity Problems of Russian Academy of Sciences, 39 Khalturin St., Ufa 450001, Russia

^BThe Shukshin Altai State Humanities Pedagogical University, Korolenko str., 53, 659333, Biysk, Russia

^CNational Research Tomsk State University, 36 Lenin Ave, Tomsk 634050, Russia

e-mail: ^A elena.a.korzniakova@gmail.com, ^B zakharovpvl@rambler.ru, ^C dmitriev.sergey.v@gmail.com

A lot of intermetallic materials having a wide gap in the phonon spectrum can support existence of intrinsic localized modes – discrete breathers (DB). Pt₃Al is an example of the material having a wide gap in the phonon spectrum due to a big mass difference of the components. Different types of DB in Pt₃Al have been excited and analyzed [1]. All these modes were investigated for the case of bulk material. However, consideration of surface effects in nonlinear dynamics is of particular importance due to the fact that any external impact inducing DB excitation in case of real materials starts from the surface. It was earlier shown for the case of graphene [2] that structure and properties of bulk and surface DBs differ significantly. In present work the analysis of surface effect and orientation on the DB dynamics and properties has been performed. A considerable effect of the surface termination layer has been demonstrated. The properties of DBs differ substantially in the case of a surface terminating with Pt atoms and Pt and Al atoms in equal proportions. The energy of the DB on the PtAl surface is substantially (three to four times) smaller than the energy in the bulk DB or the energy of the DB located near the Pt surface.

Reasons for variability of surface DB behavior are discussed.

E.A. Korznikova is grateful for the financial support from the Russian Foundation for Basic Research (grant No. 17-02-00984). P. V. Zakharov acknowledges financial support provided by Russian Science Foundation, grant No. 16-12-10175. S.V. Dmitriev thanks financial support provided by the Russian Science Foundation, grant No. 14-13-00982.

References

- [1] P.V. Zakharov, M.D. Starostenkov, A.M. Eremin, E.A. Korznikova, S.V. Dmitriev, Phys. Solid State **59**, 223 (2017) .
- [2] S.V. Dmitriev, E.A. Korznikova, J.A. Baimova, M.G. Velarde, Phys. Usp. **59**, 446 (2016)