GENERATION OF FRENKEL DEFECTS ABOVE THE DEBYE TEMPERATURE BY PROLIFERATION OF PHONONS NEAR THE BRILLOUIN ZONE EDGE

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Malte Jongmanns received his B.Sc. and M.Sc degree in theoretical physics at the University of Duisburg-Essen (DuE) in Duisbrug, Germany.

Since 2017, he has been working as a PhD student at DuE. He is involved in the German Research Foundation Priority Program on manipulation of matter controlled by electric and magnetic fields (SPP 1959). His work is focused on atomistic modeling, such as Molecular Dynamics. In particular, he is researching the mechanisms of flash sintering of ceramics and metals.

Molecular Dynamics simulations show that Frenkel pairs of vacancies and interstitials in an aluminum single crystal can be induced by the proliferation of lattice vibrations near the Brillouin-Zone edge. The simulations were performed with periodic boundary conditions along the a- and b-axis of a single crystal, and with a free surface. An EAM potential for Al was employed. The lattice vibrations near Brillouin edge were injected at different rates. The vibrations were not correlated in phase. Surprisingly we find that Frenkel interstitials are created above the Debye temperature, but much below the melting point. The molar concentration of the Frenkel pairs was 10–3 mol, which is far above equilibrium.

These results are consistent with flash experiments on polycrystals and single crystals of zirconium and titanium oxides where the Debye temperature was discovered to be the lower limit for the onset of the flash [1]. The presentation will attempt to draw a confluence between MD simulations and these experiments, even though the latter involve electrical fields while the simulations pertain only to the injection of lattice vibrations. The simulations may also be relevant to recent results on flash sintering of aluminum [2].

In summary, the present work suggests three conditions for the generation of Frenkel pairs: (i) sample temperature must be above the Debye threshold, (ii) lattice vibrations near the Brillouin Zone edge must be excited, and (iii) these vibrations must proliferate at a high rate.

[1]   D. Yadav and R. Raj. J Am Ceram Soc. 100, 5374–5378 (2017)
[2]   B. McWilliams, J. Yu, F. Kellogg, J. Mater. Sci., in print (2018)

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