Nucleating different coordination in crystal under pressure: Study of B1-B2 transition in NaCl by metadynamics

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Prediction of crystal structures has reached a high level of reliability, but much less is known about the mechanisms of structural transitions and pertinent barriers. The barriers related to nucleation of crystal structure inside another one are critically important for kinetics and eventually decide what structure will be created in experiment.

We show here an NPT metadynamics simulation scheme [1] employing coordination number and volume as collective variables and illustrate its application on a well-known example of reconstructive structural transformation B1/B2 in NaCl. Studying systems with size up to 64000 atoms we reach beyond the collective mechanism (Fig.1 (a)) and observe the nucleation regime (Fig.1 (b)). We reveal the structure of the critical nucleus and calculate the free-energy barrier of nucleation and also uncover details of the atomistic transition mechanism and show that it is size-dependent.

Our approach is likely to be applicable to a broader class of structural phase transitions induced by compression/decompression and could find phases unreachable by standard crystal structure prediction methods as well as reveal complex nucleation and growth effects of martensitic transitions.

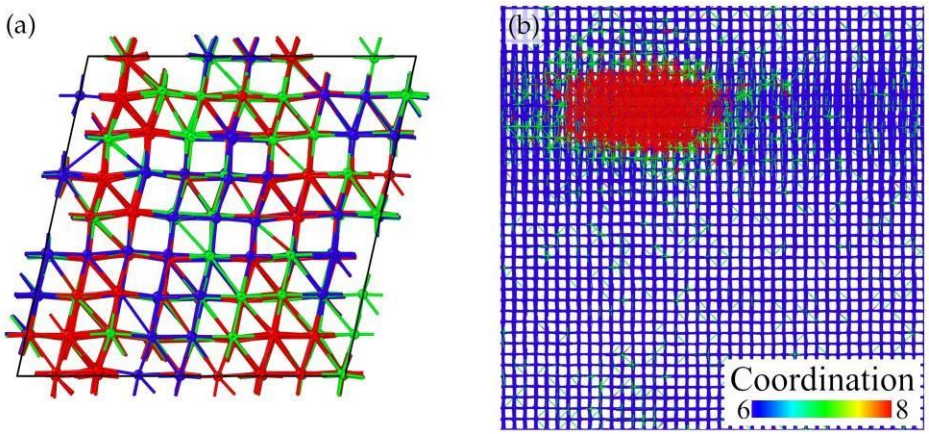

Figure 1. (a) Collective mechanism - A typical frame of supercell during the course of the B1/B2 transition in NaCl at 40 GPa and 300 K in the system of size of 512 atoms. (b) Nucleation - A typical nucleus of the B2 phase in the B1 phase (with shape of ellipsoid), during the transition at 40 GPa and 300 K in the system of 64 000 atoms. Plane of view cuts the ellipsoid through its centre. Figure was produced using OVITO [2].

1. M. Badin and R. Martoňák, arXiv:2105.02036

2. A. Stukowski, Modelling Simul. Mater. Sci. Eng. 18, 015012 (2010).

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