Molecular-Dynamics Study of Physical Properties in Sintered Nano-Particles

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Nano-crystalline metals, in which the size of grains is in the nanometer range, exhibit physical properties different from ordinary polycrystalline materials, thus these materials are of technological interest [1]. One example is the increasing hardness with decreasing grain size due to dislocation immobilisation at the grain boundaries (Hall-Petch effect). However when decreasing the grain size below a critical value, sliding processes between the grains decrease the hardness which is called the reverse Hall-Petch effect [2, 3]. Another interesting aspect is the phase stability of a polymorphic material and structural phase transitions such as martensitic transformations in Fe-based alloys [4] in nano-crystalline materials. Here we report on the first molecular-dynamics simulations [5] in combination with contact-dynamics [6]. We used the contact-dynamics method to determine the arrangement of a number of particles with a given size-distribution. Using this arrangement as the initial configuration of randomly oriented nano-particles and modeling the sintering-process on the atomic scale within the framework of molecular-dynamics simulations, where the atomic interactions were described by an embedded-atom method (EAM) potential specially designed to model the Fe-Ni alloy [8, 7] and Al [9]. After a simulation time of some 100 ps a more or less dense polycrystal has formed, whereas the density depends on the temperature and pressure. Interesting physical properties of the formed nano-phase material such as the afore mentioned reverse Hall-Petch effect and martensitic transformations were studied and compared to single-crystals.

References

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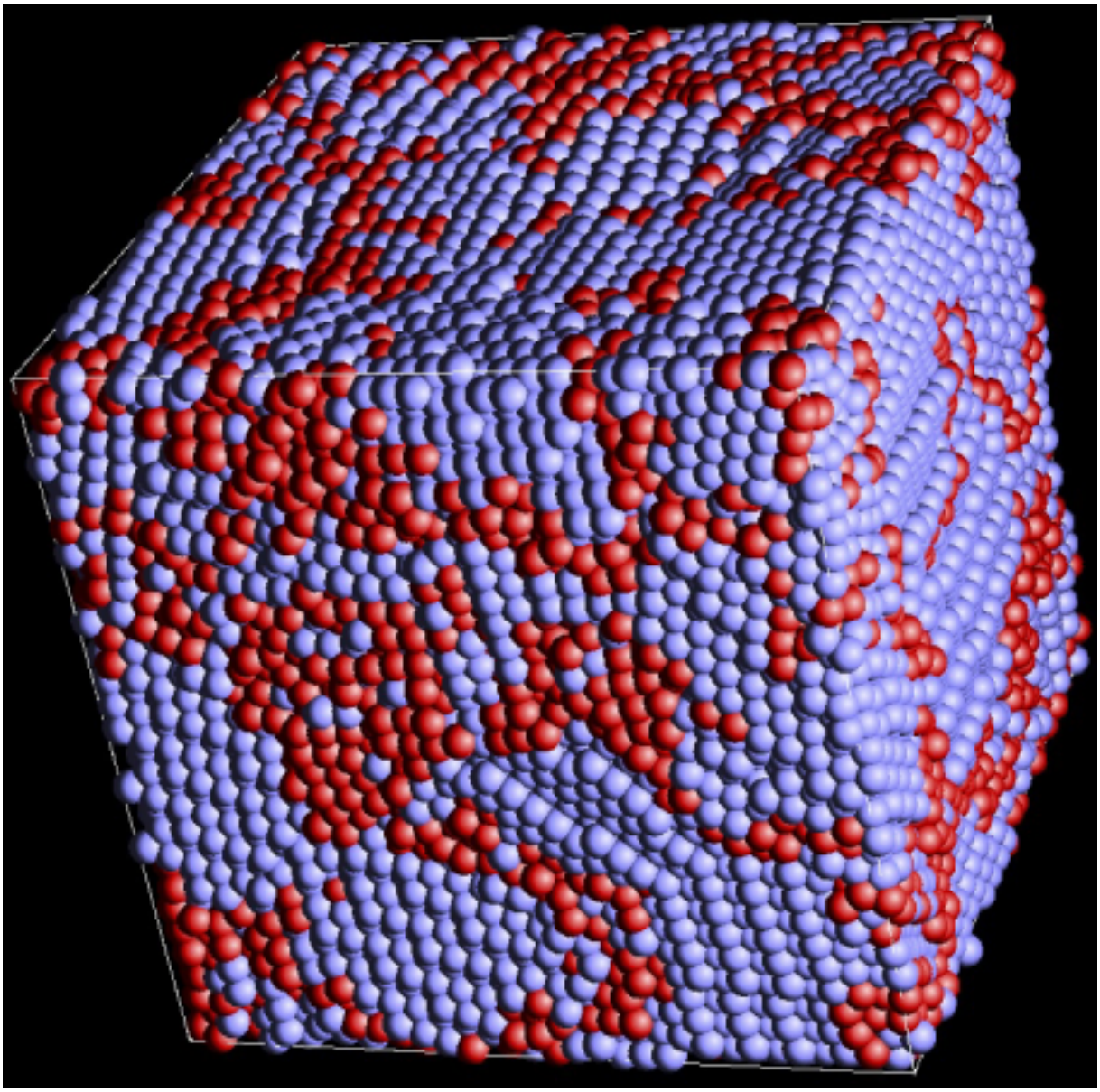

Nano-phase Aluminum after compactation of 32 fcc ordered nano-particles for 109.5 ps at 800 K and 5 GPa. Fcc structured atoms are marked bright, atoms within grain-boundaries are marked dark. Similar results were observed for $Fe_{80}Ni_{20}$ alloys. The main differences between the polymorphic $Fe_{80}Ni_{20}$ polycrystals and the Al polycrystals are the bcc ordering of the grain-boundaries and the nucleation of the martensitic bcc structure at the grain-boundaries in the alloy.