CRYSTAL STRUCTURE AS A KEY FACTOR IN THE UNIQUE PROPERTIES OF Nb_3Sn INTERMETALLICS

Taimo Priinits[1] (presenting author), Artjom Vargunin[1], Smagul Zh. Karazhanov[2,3], Aleksandr Liivand[1]

[1]*Institute of Physics, University of Tartu, 50411 Tartu, Estonia,* [2]*Department for Solar Energy Materials and Technologies, Institute for Energy Technology, NO-2027 Kjeller, Norway,* [3]*Thin film laboratories, Institute of Solid State Physics, University of Latvia, 1063 Riga, Latvia*

e-mail of presenting author: taimo.priinits@ut.ee

Two main points have been found to be very important for some micro- and macroscopic properties of Nb_3Sn intermetallic alloys with A15 structure. The first is the series of structural transformations that occur when Sn atoms are added to the pure niobium sample, see Fig. 1. We have shown that these transformations occur in such an evolutionary manner that the initial lattice structure of metallic niobium is reconstructed while maintaining the electronic structure of niobium close to the Fermi surface. Thus, the formation of specific Nb chains is a natural result of directed structural evolution. The second is the crystallographic effect associated with the point symmetry features characteristic of Nb sites in the A15 crystal structure. We predicted that the crystallographic equivalence in point symmetry of Nb sites would be removed when the alloy microstructure is formed in the form of sintered grains. Accordingly, two new types of grains will appear, which are distinguished by the network meshes composed of Nb chains.

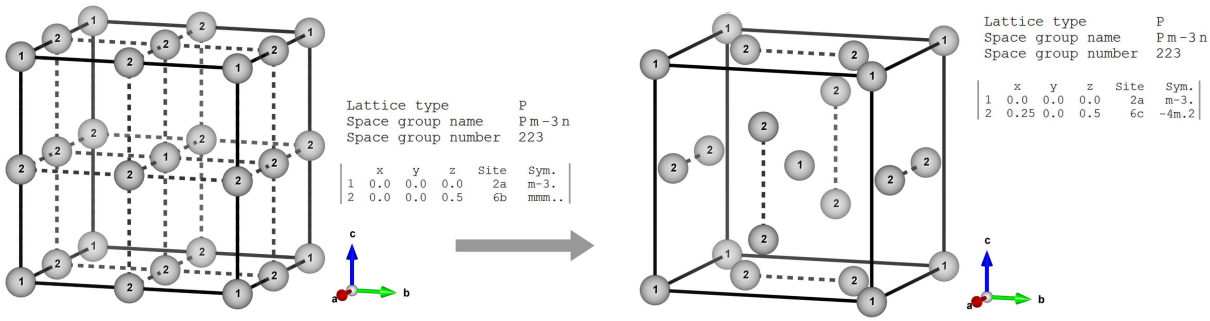

Fig.1 Reconstructive model illustrating the formation of the A-15 lattice structure for the intermetallic compound Nb_3Sn and represented in terms of point symmetry changing ($D_{2h} \rightarrow D_{2d}$) initial positions of niobium atoms. The atomic-scale reconstruction scheme is drawn in terms of off-center displacements of niobium atoms along the three main crystallographic directions of the cubic architecture. The atomistic model was constructed and simulated using DFT calculations.