

京都大学 構造材料元素戦略研究拠点セミナー

日 時: 2016年9月1日(木) 13:30~15:00

場 所: 工学部物理系校舎5階材料工学セミナー室(527室)

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講演題目: "First - principles study of nanotwin boundaries in Ni₂MnGa magnetic shape memory alloy "

Abstract:

The Ni₂MnGa magnetic shape memory alloy is very well known because it exhibits interesting properties such as giant magnetic field - induced strain (MFIS). The MFIS is related to the high mobility of martensitic twin boundaries in connection with a large magneto - crystalline anisotropy. Magnitude of the MFIS depends on the exact composition and structure of martensite and can reach up to 12 %. Different martensitic structures can be derived from tetragonally distorted L2₁ structure with and without presence of alternating sequences of nanotwins constituted of (101) planes. Structures with nanotwins (also called modulated) differ in the number of (101) planes with the same orientation or, in other words, in distances between nanotwin boundaries. Our results based on first - principles electronic structure calculations show high importance of nanotwin double layers for stabilization of modulated martensitic phases and their mutual intermartensitic transformations. Nanotwin double layers consist of two (101) planes with the same orientation and intermartensitic transformation can be understood as reorientation of these double layers to opposite twin variants.

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