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Hysteresis Design of Magnetic Materials for Efficient Energy Conversion

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Zoom information

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Interphase boundaries in thin films and bulk materials: prediction and experiment

Abstract:

The physics of surfaces and interphase boundaries contribute greatly to the properties of materials in real applications, especially when device miniaturization, reduced dimensionality and nanostructures are considered. Unlike the bulk properties, which are studied nowadays with a set of robust theoretical and experimental methods, the investigation of the structure and properties of the interfaces remains a great challenge for materials science. Mechanisms defining possible orientation relationships and habit planes between two phases are not fully known. In turn, modification of the architecture of interfaces in nanostructured bulk materials, hybrid nanoparticles and thin films is crucial for tailoring their functional properties through stresses and lattice defects induced, also stabilization of metastable phases is possible.

Here it will be discussed a combination of experimental and simulation approaches aimed to predict and examine the formation conditions and orientation relationships of interphase boundaries of stable and metastable phases as thin films. The effect of structural order and lattice stresses induced on their structural and optical and magneto-optical properties is under investigation. Beginning with a pure crystallogometrical approach proposed to predict orientation relationships, habit planes, and atomic structures of the interfaces, including atomically smooth and stepwise ones, between thin films and various substrates as well consideration of buffer layers possible between them it goes to the more precise analysis of the interface energy with classical molecular mechanics and quantum chemical calculations. The role of the substrate surface and off-stoichiometry of atomic flux, the formation of competitive phases, is used to produce thin films and tailor their functional properties. Results are given for the case of the iron, manganese silicides and MAX-phases.

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