京都大学 構造材料元素戦略研究拠点セミナー

日　時： 2013 年 11 月 15 日（金）13:30～14:30
場　所： 京都大学工学部物理系校舎（吉田キャンパス）
1 階 112 講義室

講演者：**Dr. Vaclav Paidar**
Institute of Physics,
The Academy of Sciences of the Czech Republic,
Prague, Czech Republic

講演題目: **Anisotropic behaviour of dislocations**

Abstract :
The interaction of dislocations is affected by the elastic anisotropy of materials and then the dislocation core structure may qualitatively differ in the system with the identical crystallographic lattice. This effect was studied in six B2 intermetallics with the aim to elucidate activity of different slip systems in these alloys. Moreover, the forces between dislocations are non-radial what will be demonstrated for $L1_2$ and B2 systems. It may have direct impact, for instance, on dislocation cross-slip and other dislocation processes.

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講演者：**Dr. Martin Zouhar**
Central European Institute of Technology
CEITEC MU, Masaryk University
Brno, Czech Republic

講演題目: **First-principles investigation of deformation of As, Sb and Bi and prediction of structures of epitaxial (111) and (0001) thin films**

Abstract :
We have performed an ab initio study of deformation in As, Sb and Bi along selected deformation paths. The density functional approach was applied to several crystal structures including the ground-state A7 and the cubic structures. Some of them appear on hydrostatic pressure transformation paths in case of As and Bi, and their modifications may be found along several other deformation paths. All these paths are described by three parameters: volume per atom, trigonal distortion and an internal parameter of the ground-state structure.
We calculated the total energies along these deformation paths by pseudopotential VASP code, displayed them in contour plots as functions of the above-mentioned parameters, identified energy extrema corresponding to the four basic structures and found minimum energy paths connecting selected structures. The calculated energy profiles are employed to determine the structure parameters of As, Sb and Bi thin films on various substrates with the (111) cubic or (0001) hexagonal geometry. Overall good agreement with available experimental data has been found, but we also provide many theoretical predictions which may motivate experimentalists for a deeper study of these systems.

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