TITLE:
A density functional study of total energy profiles of As, Sb and Bi along selected deformation paths applied to epitaxial thin films.

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ABSTRACT:
We present an ab initio study of structural properties of As, Sb and Bi in their A7 ground state and three cubic modifications.

The cubic structures and corresponding trigonal deformations are described using three parameters of the ground state structure A7 - atomic volume, trigonal distortion and an internal parameter 'u' of the A7 structure (for cubic structures, u=0.25).

Employing pseudopotential VASP code, we calculate the total energies along selected deformation paths, display them in contour plots as functions of the above-mentioned parameters and identify energy extrema corresponding to the four basic structures.

The calculated energy profiles are used to determine the structure parameters of As, Sb and Bi thin films on various substrates with the (111) cubic or (0001) hexagonal geometry.

An overall good agreement with available experimental data motivates us to provide many theoretical predictions which may challenge experimentalists for a deeper study of these systems.