Contribution ID: **506** Type: **Poster Presentation**

Computational studies of the bulk cobalt pentlandite (Co₉S₈): Validation of the potential model.

Tuesday, 9 July 2013 17:40 (1 hour)

Abstract content
   (Max 300 words)

We investigate various forms of the cobalt pentlandite, Co₉S₈, at different temperatures, using classical atomistic simulation methods with the support of electronic structure calculations. The first interatomic potentials of Co₉S₈ based on the Born model, were derived with input data such as structure and elastic properties from experiments and electronic structure calculations respectively. The interatomic potentials were validated by running energy minimization and molecular dynamics calculations. The structure, elastic properties and phonon spectra corresponded well with those determined by electronic structure methods. The calculations further reproduced the complex high temperature transformation to high form pentlandite and the melting of Co₉S₈; as deduced from the crystal structure and radial distribution functions. The interatomic potentials can be used for studies of surfaces and nanostructures.

Apply to be
 considered for a student
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No

Main supervisor (name and email)
and his / her institution

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Would you like to
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Yes

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