SCIENCES SORBONNE UNIVERSITÉ

2019-2020

Master thesis proposal

Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie

Campus Pierre et Marie Curie
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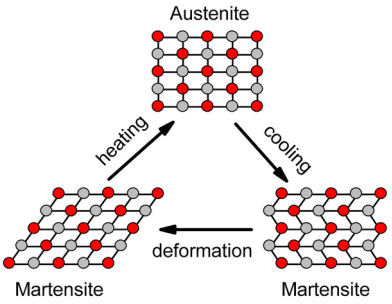
Title: Ab-initio phase transition of Nickel-Titanium alloys

Keywords: phonons, anharmonicity, phase transition, ab-initio, quasi-harmonic

Scientific description:



Nickel titanium, also know with the commercial name "Nitinol" exhibits unique memory shape effect (SME) and superelasticity (SE) properties. These properties are caused by the presence of two similar phases: low-temperature low-symmetry martensite phase which has the lowest electronic energy, and a high-temperature high-symmetry austenite phase that is stabilized by thermal phonons.
The existence of two competing phases can indicate the emergence of interesting anharmonic properties, such as extremely low lattice-driven thermal conductivity which can be of industrial interest. However until today only classical force-filed molecular dynamic studies have been published.[1]
The aim of this proposal is to study ab-initio the electronic, and vibrational properties of this material in the harmonic, quasi-harmonic and anharmonic frameworks. Step 1: correctly reproduce the two phases lattice parameters, electronic structure (band dispersion, Fermi surface) and phonon dispersion. Step 2: study the phase transition in the quasi-harmonic or, if necessary, self-consistent harmonic approximations. Step 3 (optional): study the anharmonic behaviour, phonon-phonon and electron-phonon interactions or other physical properties depending on the results of steps 1 and 2.

[1] A.V. Verkhovtsev et. al., Comp. and Theo. Chem 1021 (2013) 101–108

Techniques/methods in use: ab-initio simulations
Applicant skills: fundamentals of solid state theory, running computer simulations
Industrial partnership: No

Internship supervisor(s) (name, email, phone, webmail):
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Possibility for a Doctoral thesis: Y