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.


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):
Lorenzo Paulatto, 01 44 27 98 22
lorenzo.paulatto@sorbonne-universite.fr

Internship location:
Institut de minéralogie, de physique des matériaux et de cosmochimie

Possibility for a Doctoral thesis: Y