

# Lattice dynamics of magnetic 3d metals within the KKR Green's function method

S. Mankovsky and H. Ebert

Dept. Chem./Phys.chem., LMU Munich, Germany

We present a formalism for the calculation of the force-constant tensor within the KKR Green's function method. As a primary information the formalism gives the real-space force-constant tensor, i.e. the pairwise interaction parameters, on the basis of ab-initio electronic structure calculations. Accordingly, the technique is applicable in principle to any system as for example solids, surfaces and nanostructures.

First results of calculations of the force-constant tensor as well as phonon spectra of magnetic metals and alloys will be presented. The influence of magnetism on the elastic properties as well as phonon spectra will be analysed. The calculated phonon spectra were used to investigate the role of magnetism in structural stability of 3d transition metals and alloys.

← 13.4 cm →

## Subject category :

6. Soft and Hard Magnetic Materials

## Presentation mode :

poster

## Corresponding author :

Dr. S. Mankovsky

## Address for correspondence :

Dept. Chemie und Biochemie/Phys.Chemie, Universität München, Butenandtstr. 5-13, D-81377 München, Germany

## Email address :

sergiy.mankovskyy@cup.uni-muenchen.de

9.7 cm