On the phonon excitations of rich borides: phenomenological modelling and neutron inelastic scattering experiments

D.V. Sedyakina[1,2], **E.S. Clementyev**[3]

[1] Joint Institute for High Temperatures RAS, Izhorskaya 13 bldg. 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskii per. 9, Dolgoprudny, Moscow 141700, Russia
[3] Institute for Nuclear Research RAS, prospekt 60-letiya Oktyabrya 7a, Moscow 117312, Russia
*sedyakina.d@gmail.com

1. Introduction

This work is aimed to study lattice dynamics in YbB_{12} and SmB_6. These rich borides are typical members of the class of materials broadly known as Kondo-insulators. This term denotes compounds which are close to valence instability and become semiconducting with a narrow energy gap at low temperature [1]. We use a Born-von Karman force-constant phenomenological model to describe these materials and compare obtained results with the inelastic neutron scattering (INS) experiments [2].

2. The structure of YbB_{12} and SmB_6

The crystal lattice of YbB_{12} is a variant of the NaCl structure, with boron cuboctahedron instead of chlorine (see Fig. 2). The crystal lattice of SmB_6 is similar to the CsCl structure and consists of samarium atoms and boron octahedra (see Fig. 1). In our modeling boron clusters are replaced by pseudo atoms with the mass of the corresponding cluster (see Figures 1–2 right).

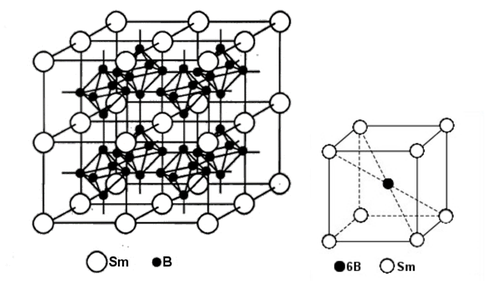

Figure 1: *Crystal structure of SmB_6: space group Pm3m, lattice constants $a = 4.135\AA$, distance between nearest boron atoms $d_{B-B} = 1.76\AA$.*

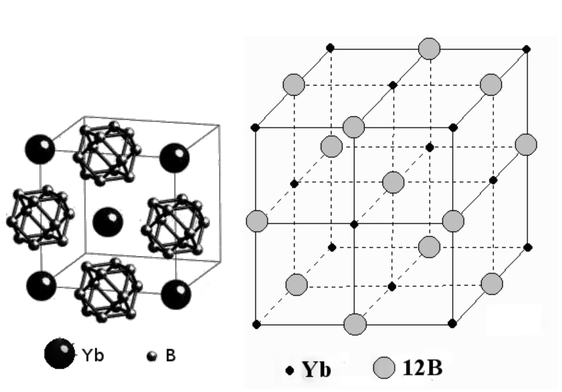

Figure 2: *Crystal structure of YbB_{12}: space group Fm3m, lattice constants $a = 7.468\AA$, distance between nearest boron atoms $d_{B-B} = 1.71\AA$.*

3. Theoretical description

In this work lattice dynamics is considered in case of small displacements of the atoms from their respective equilibrium positions. Modelling the vibrational properties of a crystal within the harmonic approximation implies the construction of the force constant matrix [3]. We use Born-von Karman model for this purpose. In terms of this model each interraction is defined by Longitudinal force constant and Transverse force constant. These constants are treated as model parameters and they are not interpreted in terms of a special interatomic potential.

4. Phenomenological modeling

We obtained dispersion curves for simplified structure using the UNISOFT software package [4]. Values of longitudinal and transverse force constants used for simulation and atomic positions in the primitive cell in UNISOFT notation are listed in Tables 1 and 2. Force constants are chosen so that the results of modeling correspond to the data on INS experiments [2]. It turned out that a simple approach with pseudo atoms can reproduce with good precision the dispersion of longitudinal, transverse acoustic modes and significant lower part of the optical modes for frequencies up to 10 Hz (i.e. energy up to ~ 40 meV) (see Figures 3–4).

The values of the force constants demonstrate a hierarchy of interactions, the B-B interaction is the most strong and the Yb-Yb (Sm-Sm) interaction - the weakest. Lattice dynamics at high frequencies can't be reproduced with a simplified model. It does not account for intrinsic degrees of freedom of cubic boron octahedra and cuboctahedron fluctuations occurring at high energies due to the strong interraction of boron-boron and a small mass of boron atoms. Based on the results for dispersions phonon density of states of higher borides samarium and ytterbium were calculated [5] (see Figures 5–6).

Table 1:

SmB_6	Sm-B	Sm-Sm	B-B
Longitudinal	40	-1.5	900
Transverse	-8	-1.5	100
Atomic positions	Sm (0.5; 0.5; 0.5) B (0; 0; 0)		

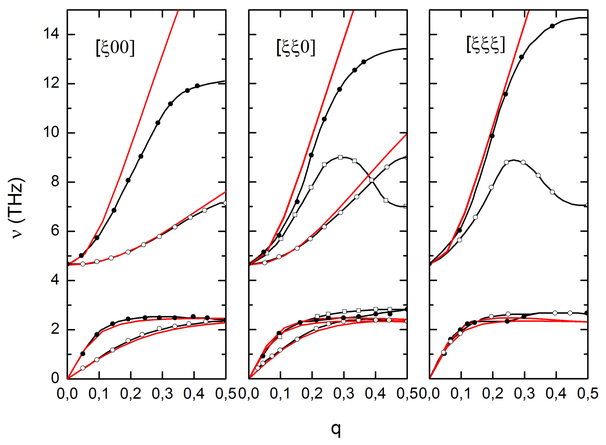

Figure 3: *Phonon dispersion curves in SmB_6 along main symmetry directions, red solid lines correspond to the results of modeling with pseudo atoms, dots and black solid lines correspond to the data on INS experiments.*

Table 2:

YbB_{12}	Yb-B	Yb-Yb	B-B
Longitudinal	-2	-1	2
Transverse	35	-1	100
Atomic positions	Yb (0; 0; 0) B (0.5; 0.5; 0.5)		

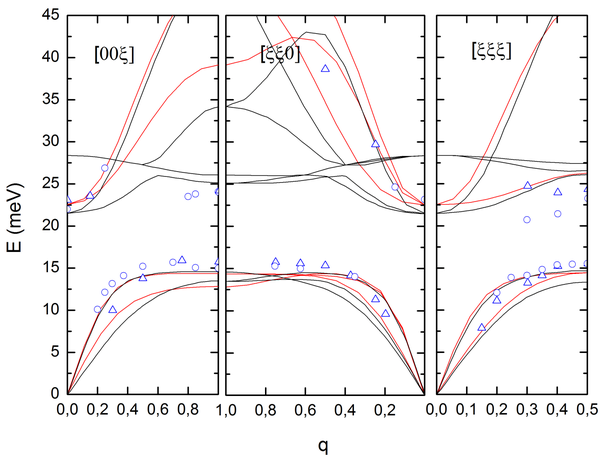

Figure 4: *Phonon dispersion curves in YbB_{12} along main symmetry directions, red solid lines correspond to the results of modeling with pseudo atoms, dots and triangles correspond to the data on INS experiments, black solid lines - modeling of the true YbB_{12} structure.*

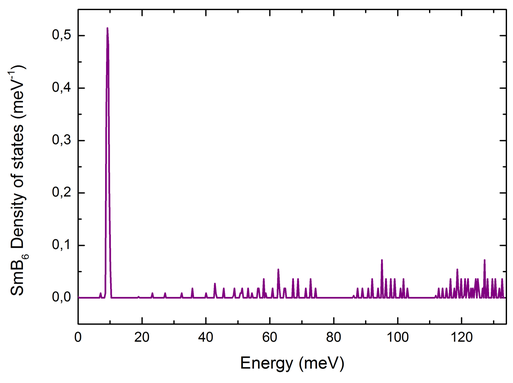

Figure 5: *Density of states for SmB_6 structure with pseudo atoms.*

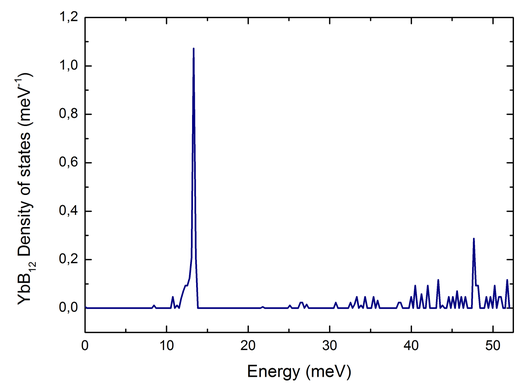

Figure 6: *Density of states for YbB_{12} structure with pseudo atoms.*

In turn, the lattice contribution to the heat capacity was obtained on the basis of the phonon spectra and the phonon density of states (see Figures 7–8). It can be considered that values of the specific heat are reliable at low temperatures [6].

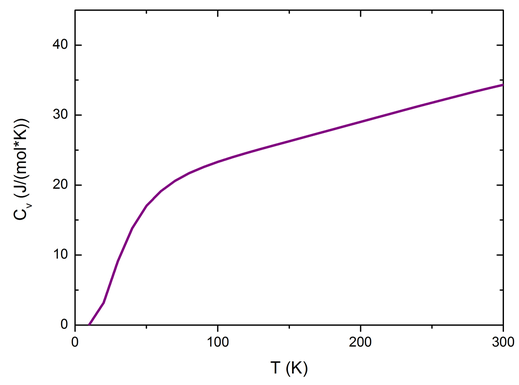

Figure 7: *The temperature dependence of specific heat of SmB_6 in modelling with pseudo atoms.*

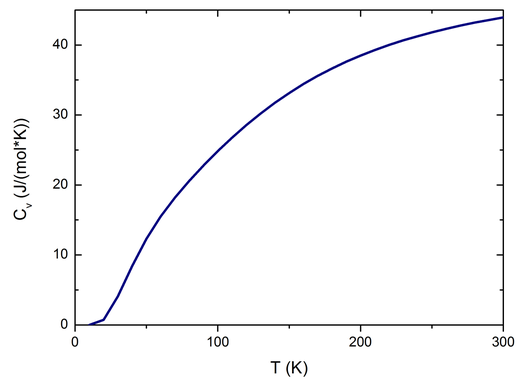

Figure 8: *The temperature dependence of specific heat of YbB_{12} in modelling with pseudo atoms.*

5. Conclusions

1. Resulting dispersion curves are in good agreement with the data on the phenomenological calculation based on the true structure of borides and INS experiments for frequencies up to 10 THz.
2. Lattice contribution to the specific heat at low temperatures is in good agreement with the experimental data.
3. Pseudoatomic phenomenological model can be successfully used for the analysis of some physical properties of rich borides.

References

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