

Project Title:

Quantum phase transition of Chromium (Cr) under high pressure

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1. The spin density wave (SDW) of Chromium under high pressure is studied by the first principle calculation. The bcc chromium is typical itinerant electron system, and it presents continuous quantum phase transition induced by tunable electronic correlation under high pressure. This project is funded by Grant-in-Aid for Scientific Research on Innovative Areas 'Earth science based on the high pressure and temperature neutron experiments' (No. 20103001-20103005) from the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan.

2. The derivation of propagation vector and the Fermi surface of Chromium under high pressure are studied by VASP, PWSCF and Wien2k. It is widely accepted that the wave vector of SDW state is determined by the nesting Fermi surface. Our study on the nesting vector predicates that this mechanism is not true, since the calculated nesting vector doesn't agree with the experimental results very well.

3. The computational results also show the magnetic structures of Cr are very sensitive to the lattice constant and the choice of the Hubbard U parameter. The electronic of the magnetic phases at ambient pressure can be described adequately with the spin-polarized local density approximation with a small effective Hubbard parameter. The effect of increase electron correlation at high pressure mimic by larger U values helps to rationalize the recently observed quantum phase transition.

4. From above calculation, we think that the SDW state in the Cr is not only due to the instability of Fermi surface, but the instability of Fermi Sea.

RICC Usage Report for Fiscal Year 2009

Fiscal Year 2010 List of Publications Resulting from the Use of RICC

[Publication]

[Proceedings, etc.]

[Oral presentation at an international symposium]

Spin Density Wave in Chromium under High Pressure, Zhi Li, John S. Tse, Toshiaki Iitaka,
The 5th Asian Conference on High Pressure Research (ACHPR-5)

[Others]