

Muon sites in Ce(Ru, Rh)₂Al₁₀ investigated using Density Functional Theory from the perspective of electronic potential[†]

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CeRu₂Al₁₀ has the orthorhombic YbFe₂Al₁₀-type structure with space group Cmcm.¹⁾ Ce atoms control the magnetism of this system and are surrounded by Al atoms forming a cage-like structure which is suggested to form a two-dimensional plane structure stacking along the *b*-axis.^{2,3)} Despite having the nearest neighbour distance, approximately 5.2Å between Ce ions, CeRu₂Al₁₀ exhibits an antiferromagnetic transition at $T_0 = 27.3$ K which cannot be explained by taking only RKKY interaction into account.⁴⁾ The magnetic susceptibility is largely anisotropic whereas the direction of magnetic moment is along the *c*-axis and is expected to flip to the *a*-axis when a small concentration of Ru atoms are substituted by Rh atoms.⁵⁾ In addition, from the μ SR results of a Rh-doped system, Guo et al. reported drastic changes in internal fields at muon sites which were related to the spin-flop caused by doping of 3% Rh atoms in CeRu₂Al₁₀.⁶⁾

A number of investigations of muon sites in Ce-based Kondo semiconductors, CeRu₂Al₁₀ and Ce(Ru, Rh)₂Al₁₀ were carried out by using Density Functional Theory (DFT) to understand the magnetic properties. From the calculation of electrostatic potential, we found all muon sites previously suggested by Kambe et al.⁷⁾ and Khalyavin et al.⁸⁾ as shown in Figure 1. Because they were not crystallographically identical, muon sites in CeRu₂Al₁₀ are still undefined and the hyperfine interactions cannot be discussed in detail.

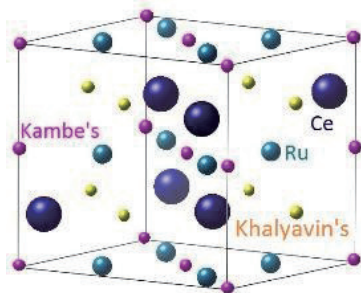


Fig. 1. Muon sites in CeRu₂Al₁₀ suggested by Kambe et al.⁷⁾ and Khalyavin et al.⁸⁾

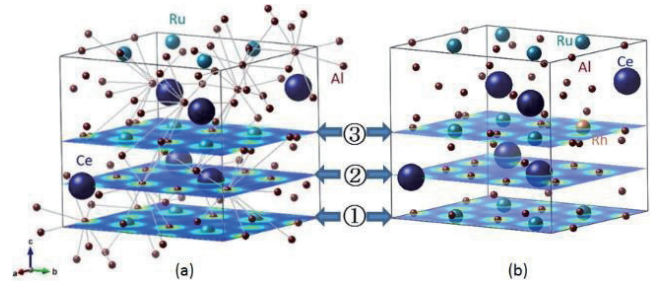


Fig. 2. Three planes that differentiate CeRu₂Al₁₀ (a) and Ce(Ru, Rh)₂Al₁₀ (b). Planes (1) and (3) contain the muon sites suggested by Kambe et al., whereas the plane (2) contains the muon sites suggested by Khalyavin et al. In plane (3), one Ru atom is substituted by one Rh atom.

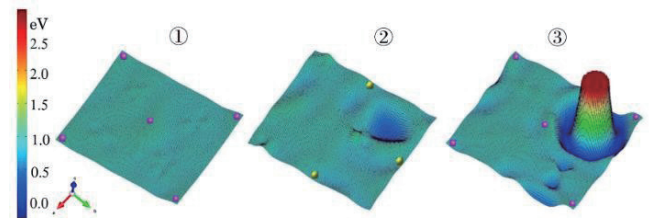


Fig. 3. Potential differences between non-doped and doped systems in planes (1), (2) and (3). The purple and yellow points on the planes indicate the positions of suggested muon sites.

The potential energies calculated for the plane in the non-doped system were subtracted from those of corresponding plane in the doped system to investigate the potential differences. Large differences are seen in plane (3) where a Ru atom was substituted by a Rh atom. Because of this change at the Rh atom in plane (3), the potential energy in plane (2) is also slightly deformed around the position underneath the Rh atom. The large potential difference at the substituted Rh atom in plane (3) may have been because of the difference in valence configuration from that of Ru atom.

However, the potential energy at the suggested muon sites did not exhibit much difference even though the Rh doping concentration in the CeRu₂Al₁₀ was increased to 12.5%.

References

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