Electronic States and Transport Properties of Semiconductor-Semimetal Heterostructures

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Semimetallic rare-earth (RE) pnictides are candidates in which the optical properties can be contralled by tuning the electronic states near Fermi level by using superlattices, heterostructures and/or quantum-dot structures. Recent STM measurements for ErP dots suggest that a change from semimetallic(SM) to semiconducting(SC) state occurs by reducing the size of ErP systems [1]. In order to understand the relation between the electronic states and measured results, we adopt a simple model for of a heterojunction of doped-SC/SM/doped-SC and study the dependence of the resistance on the electronic structure and system size.

An example of calculated results is shown in Fig. 1, where the resistance of the heterojunction is plotted as a function of ΔE, a difference between the top of the valance band and the bottom of the conduction band of a bulk semimetal. A schematic figure of the electronic states is shown in the inset. Here, the hopping integral (~0.5eV) between the nearest neighbor sites is taken as the unit of energy. Because we adopt a finite size junctions with a simple cubic lattice, the cross section of which is 12 times 12 and the thickness of the SM layer is 5, the cross-over from SM to SC occurs at ΔE~0.2. We find the increment of the resistance is maximal at this value of ΔE.

Another interesting RE-related materials are Er doped SCs, in which optical luminescence from Er *f*-states is modulated by the presence of SC atoms surrounding Er atoms. In a case of transition metal (TM) doped magnetic SCs, the *d*-levels of TM strongly mix with *s*-*p* bands of SC and show characteristic level structures due to a presence of the energy gap of SCs [2]. On the other hand, 4*f*-states of RE elements are corelike states and may mix much less with *s*-*p* bands. The energy level splitting of 4*f*-levels is thus much smaller as compared with 3*d*-states. The orbital dependence of level splitting might be interesting to compare with the photo luminescence, which will be presented in the Poster session.

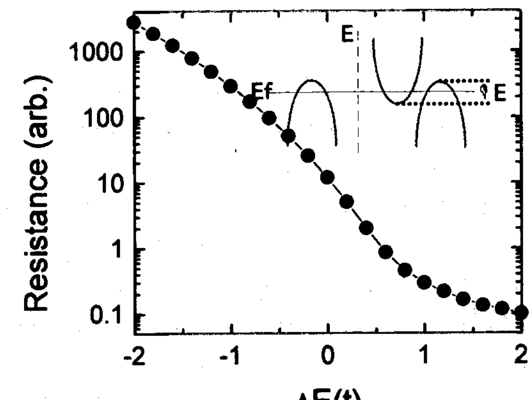

Fig. 1. Resistance vs ΔE defined in the inset for a semiconductor/semimetal heterojunction. A crossover from semimetal to semiconductor occurs at ΔE~0.2*t*, where *t* represents a nearest neighbor hopping integral.

References

[1] L. Bolotov et al., Phys. Rev. **B59** 12236 (1999).
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