

Optical properties of ErH_{2+x} : First principles calculations and experimental measurements

Rare earth and transition metal hydrides exhibit many interesting physical phenomena, from metal-semiconductor transitions to transparency changes at RT as a function of hydrogen content. Electrical resistivity measurements by P. Vajda (1) indicate that ErH_{2+x} undergoes a metal-semiconductor transition between 240-290K and an antiferromagnetic transition between 1.75-2.3K depending on hydrogen content. These same transitions should also cause profound changes in the optical properties. This work will present first principles calculations of the optical properties of ErH_{2+x} from 300-600K where x ranges from -0.2 to 0.2. The calculations will be compared to experimental results on thin films of ErH_{2+x} which were obtained as a function of temperature from 10-600K and hydrogen content.

(1) P. Vajda and J.N. Daou, Phys. Rev. B., Vol. 49, p. 3275 (1994).

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