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# Optical properties of solids by ultra-high vacuum spectroscopic ellipsometry

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The optical conductivity spectra of various metals and alloys were measured in the energy range of 1.5 to 5.4 eV using ultra-high vacuum (UHV) spectroscopic ellipsometry. The ellipsometer was rotating-analyzer type and a pair of low-retardance fused-quartz windows were used to reduce the stress induced birefringence due to non-uniform tightening of the windows.

We investigated the isostructural phase transition of metallic α- and γ-Ce. The samples were thin films deposited *in-situ* by evaporation of high-purity Ce on sapphire substrate at room temperature and 25 *K* for γ- and α-Ce, respectively. The sample holder and substrate were cooled with a closed-cycle helium refrigerator. α-Ce prepared in this way contains a negligible amount of γ-Ce. The UHV chamber pressure was kept below $2x10^{-9}$ Torr during deposition and below $2x10^{-10}$ during measurements.

The thin films were repeatedly doposited on top of previously deposited films to study the thickness dependence of the optical conductivity. The measured conductivities decrease in magnitude as the film thickness increases. Since the magnitude of optical conductivity decreases as film grows, we argue that the sample becomes rougher as it grows. In order to check this point we used three-phase model in which the overlayer was consists of bulk Ce and the void, and the overlayer thickness *d* and the volume fraction of void *f* were used as adjustable parameters. In this microscopic surface roughness model we employed the Brugemann effective medium approximation since it treats all media on an equal footing. Both the overlayer thickness and the void fraction increased as the film thickness increased. It was also consistent with the fact that the surface of α-Ce deposited on the cold substrate was rougher than that of γ-Ce because of low adatom surface mobility.

The optical conductivity increases upon entering the α-phase because of the increased number of electrons per unit volume due to the volume collapse. The volume of the α-phase is about 17% smaller than the γ-phase. The difference between the optical conductivities times the unit cell volume showed an oscillator strength change in the phase transition. The energy band structures and the optical conductivities were calculated by the linearized-augmented-plane-wave method within the density-functional theory, treating both $4f$ and $5p$ electrons as bandlike. The application of the partial sum rule to angular-momentum-decomposed optical conductivities shows that the $4f$ electron contributions in the measured energy range is small.

The optical conductivities of $CeSn_3$ and $LaSn_3$ were measured. Since they are very reactive with oxygen, UHV ellipsometry is crucial to the correct optical measurements. The chamber pressure were kept below $5x10^{-7}$ Torr for the first measurement at room temperature and the chamber was then baked out at 110C for one day. After baking the chamber pressure was below $7x10^{-10}$ Torr. We made four measurements at intervals of a day or two. The successive measurements showed reduced magnitude in the optical conductivity because of the increased oxide overlayer thickness. If the oxide overlayer is not too thick we can estimate its effects and deduce the optical conductivity of the bulk without the oxide overlayer to the first order of $d/\lambda$, where $d$ is the thickness of the oxide overlayer and $\lambda$ is the wavelength of the incident light. The conductivity partial-sum rule applied to the measured spectra gives 0.54 electrons per formula unit more for $CeSn_3$ than for $LaSn_3$. While some differences in the contribution from $d$->$f$ transitions were shown in the theoretical calculations, they are suspect because the standard local density approximation does not place the $f^2$ final state configuration at the appropriate energy.

We measured the optical conductivity of Ce using UHV spectroscopic ellipsometry. The sample preparation and measurements were made *in situ*. The dependence of the optical conductivity on the sample thickness was understood as increased surface roughness of the repeated depositions. The optical conductivities of $CeSn_3$ and $LaSn_3$ were also measured and the effects of the oxide overlayer were successfully corrected. The $f$ electron contributions to the optical conductivity was small in both cases.