E_{2g} phonon self-energies in HCP transition metals at high pressure

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Our previous Raman measurements have found the strong hardening and anomalous broadening of the E_{2g} phonon lines upon cooling in a number of transition metals with hexagonal close-packed structure (D_{6h}^4space group). In such metals as Re and Os the phonon energies (120 and 165 cm^{-1} at room temperature) increase by 8-10 cm^{-1} and simultaneously the linewidths grow by 4-6 cm^{-1} [1, 2] when temperature decreases from 600 to 5K. Although the increase of the phonon frequency can be interpreted as a manifestation of anharmonic interactions the growth of the phonon damping implies the effects of electron-phonon coupling are important. Another evidence of the strong electron induced effects are a drastic softening of the [LO] phonon branch near Γ in Re [3] and the observation of "extra" lines in Re Raman spectrum for wave vector direction along hexagonal axis [4] indicating a superstructure existence. Since different phase transformations (structural or electronic type) can be induced at high pressures and anharmonic effects may be studied for comparatively large volume changes Raman scattering investigation of transition metals Re and Os has been started and here the first results are presented.

A gasketed diamond anvil cell was used to generate high pressures at room temperature. The cleaved crystal plates of both metals having mirror basal planes with dimensions 0.2*0.2*0.05 mm^3 were surrounded in gasket hole by a 4:1 mixture of methanol: ethanol. The exciting laser lines were 4880 Å and 5145 Å with power about 100 mW in a spot of ~ 20 μm in diameter inside the cell. Ruby was used for pressure determination. Cooled photomultiplier with photon counting electronics was used to detect the backscattered light after passing through a double grating monochromator (DFS-24). Hydrostatic pressure up to 50 kbar was produced leading to a volume change for Re and Os of roughly - 1% whereas the total volume changes of these metals in going from helium to room temperature are ~ 0.4%.

With increasing pressure first-order E_{2g} Raman peaks in both metals shift to higher energies (by ~ 1.5 - 2 cm^{-1} at 40 kbar) and their frequencies show approximately linear dependence vs pressure. Estimated from the least-squares fit to the data and compressibilities mode-Grüneisen parameters γ's were found to be ~ 2 for Re and ~ 1.2 for Os. The obtained γ value for Re is smaller than calculated [5] room temperature effective Grüneisen parameter $\gamma_{\perp} = 3.08$. There are no data concerning γ for Os. Using obtained γ's the contributions of thermal expansion effect to the phonon hardening upon cooling from 300 to 5K were estimated to be ~ 1 cm^{-1} for Re and 0.8 cm^{-1} for Os in contrast to the observed frequency shifts ~ 4-5 cm^{-1}. The additional energy shifts supposed to be due to electron-phonon effects rather than to contribution of anharmonic interactions. Really, the phonon linewidths at high pressure didn't change within 0.5 cm^{-1} indicating the absence of anharmonic effects. The observed anomalous decrease of the phonon damping upon heating accompanied by small found volume effects in phonon energies should be attributed to the thermal smearing of the electronic volume states near Fermi level which mainly determine wave vector dependent effects in the phonon width and frequency renormalization at low temperatures [6].

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