Reply to "Comment on 'Optical properties of $Nd_{1.85}Ce_{0.15}CuO_4$'"

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The nature of the phonon screening is discussed for the cuprate superconductor $Nd_{1.85}Ce_{0.15}CuO_4$ that we have previously examined [Phys. Rev. B **56**, 5525 (1997)] in order to reply to the preceding Comment; the implications for phonon assignments are also examined. [S0163-1829(98)03846-6]

In their Comment[1] on our recent article[2] on the optical properties of $Nd_{1.85}Ce_{0.15}CuO_4$ (NCCO), Calvani, Capizzi, and Lupi disagree with some of the phonon assignments and suggest that in fact *no* phonons should be observed in NCCO due to screening effects. The authors then propose that any modes which are observed may be explained by a coexistence of phases and local vibrations.

The authors have raised an interesting possibility. However, there are several problems with their argument. The claim that NCCO is a "good metal" and that the infrared-active phonons should be screened is difficult to support. First, the family of cuprate superconductors are doped antiferromagnetic insulators which are "bad metals" with relatively low carrier concentrations, and display non-Fermi-liquid behavior.[3,4] Even granting that the normal-state properties resemble a Fermi liquid, the low value for the plasma frequency $\omega_p \approx 1.2$ eV (Ref. 2), where $\omega_p^2 = 4\pi n e^2/m^*$, when compared to a good conductor such as Al with $\omega_p \approx 15$ eV (Ref. 5) implies that the carrier concentration n in NCCO is more than two orders of magnitude less than in Al (assuming equivalent effective masses m^*). Given these circumstances, it seems unlikely that lattice modes will be screened effectively in NCCO or any other cuprate system.

The four infrared-active E_u modes have been unambiguously determined at ≈ 130, 305, 350, and 510 cm^{-1} in the undoped insulator Nd_2CuO_4 (Refs. 6,7); the first mode is weak, while the latter three are strong. Of the three strong modes observed in the reflectance and $\sigma_1(\omega)$ of NCCO at ≈ 303, 440, and 564 cm^{-1} at room temperature, shown in Fig. 1, the feature at ≈ 303 cm^{-1} is clearly identified as the $E_u(2)$ mode.[2,6] This presents a problem for Calvani, Capizzi, and Lupi; if the E_u mode is screened, then this mode should not be observed. If this E_u mode is observed because of phase separation, and the two high-frequency modes are actually local modes,[8] then the other E_u modes should also still be observed. To try and resolve these problems, we proposed that the difference in frequencies is a response to Ce doping and the change in valence from Nd^{3+} to Ce^{4+}; this argument has already been outlined elsewhere[2] and will not be repeated here, except to mention that this approach was motivated by the observation that the position of the high-frequency Cu-O vibration in perovskite materials is quite sensitive to coordination and doping.[9]

The introduction of Ce leads to a loss of inversion symmetry that can result in a mixing of the *in-plane* infrared and Raman modes. The speculation that some of the fine structure that is observed at low temperature in the NCCO material may be due to c-axis phonons which are activated by a *charge-transfer* mechanism (first outlined by Rice,[10] and later expanded upon by Bozio, Meneghetti, and Pecile[11]) is based on an established and well-understood mechanism to explain the anomalous optical properties of the one-dimensional organic conductors where the totally symmetric a_g vibrations, active *perpendicular* to the chain directions in these materials, are observed *along* the chain directions.[12,13] These ideas have recently been applied to the two-dimensional charge-density-wave material η-Mo_4O_{11} (Ref.

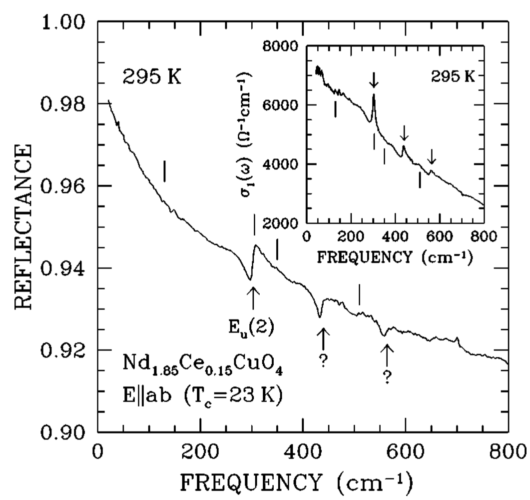

FIG. 1. The reflectance of $Nd_{1.85}Ce_{0.15}CuO_4$ (NCCO) from ≈ 40 to 800 cm^{-1} at 295 K for radiation polarized in the a-b plane. The positions of the infrared-active E_u modes in the undoped insulator are indicated by the vertical lines, while the arrows denote the fitted positions in the NCCO sample. Inset: the real part of the optical conductivity over the same frequency range, for the same temperature and polarization.

14) and lightly doped $La_{1.96}Sr_{0.04}CuO_4$ (Ref. 15).

In summary, while Calvani, Capizzi, and Lupi have raised an important point, it seems likely that the infrared active modes are not screened in the cuprate systems, and NCCO in particular. The difficulties associated with detailed phonon assignments in the doped materials will only be resolved with a detailed doping study in the metallic regime, which is underway.

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