COMMENTS

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

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A recent paper by Homes *et al.* [Phys. Rev. B **56**, 5525 (1997)] reports reflectivity spectra of superconducting $Nd_{1.85}Ce_{0.15}CuO_4$ with narrow far-infrared lines superimposed to a Drude-like term. We disagree with the assignment proposed by the authors for those lines and we suggest an alternative interpretation.
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Infrared reflectance data collected on one single crystal of $Nd_{1.85}Ce_{0.15}CuO_4$ (NCCO) ($T_c = 23$ K) have been published recently by Homes *et al.*[1] Even if the authors mainly discuss the broad anomalous-Drude absorption in this superconducting compound, they also report several sharp lines superimposed to the Drude band. The explanation they propose for these lines deserves comment. Homes and co-workers assume that the three strongest lines they observe at room temperature, at ~ 303, 440, and 564 cm^{-1}, coincide with three of the four E_u phonon modes. The authors remark that different values previously reported for the E_u modes in Nd_2CuO_4 refer to low-temperature measurements (≈ 10 K), and therefore they seem to explain such disagreement in the values of the E_u phonon frequencies in terms of large phonon shifts as T decreases, likely due to strong lattice distortions. In order to assign other lines they observe, the authors mention that the out-of-plane substitution of Nd atoms with Ce atoms causes a reduction of symmetry which results in more general selection rules. Therefore, vibrations which are active only along one polarization of the incident electric field in the undoped material, would become active also for other polarizations in the doped material. On the same grounds, Raman modes polarized both in the a-b plane and along the c axis of the tetragonal structure of NCCO would become infrared active. This would account for the observation of a number of additional weaker lines at low T's.

Several objections can be raised to the above interpretation of Homes *et al.* As far as the possibility of large phonon shifts with temperature and doping is concerned, the authors themselves report that the modes at ~ 303, 440, and 564 cm^{-1} are independent of temperature, see Fig. 2 and Table I in Ref. 1. The same holds for the lines generally attributed to E_u modes at ~ 314, ~ 352, and ~ 514 cm^{-1} in stoichiometric as well as in oxygen deficient Nd_2CuO_{4-y}.[2–5] Moreover, in three $Nd_{1.96}Ce_{0.04}CuO_{4-y}$ Ce doped samples with different oxygen concentrations y, the three E_u modes at higher energies are found once more at 304, 350, and 514 cm^{-1} and their energies change with temperature by a few cm^{-1} at most.[6] This observation also rules out the possibility that doping might be responsible for large shifts in the E_u mode energies.

As far as the possible activation of other modes is concerned, the substitution of out-of-plane Nd with Ce causes a loss of inversion symmetry in the unit cell. Raman modes with any wave vector can then become infrared active, but they would produce broad and weak bands, hardly visible on the top of a Drude band. Finally, according to group theory, vibrations along the c axis can be detected by radiation polarized in the a-b plane, only if the crystal has a monoclinic cell. In no way can the lattice disorder do the job, unless it induces structural transitions that have never been reported for NCCO by changing either temperature or doping. Therefore, the attribution of lines in the a-b plane to c-axis vibrations is not supported by solid arguments in Ref. 1.

We can add the general remark that the observation of extended phonon modes in a metal, even as poor as NCCO may be, is unlikely for the screening effect of the carriers. As a matter of fact, in good quality NCCO with $x = 0.15$ or 0.20, no evidence of extended or localized phonons has been reported previously (see Refs. 2 and 3, respectively). On the other hand, in Table I of Ref. 1 one can find at 10 K four lines, at 130.8, 304.3, 347.2, and 519.9 cm^{-1}, which coincide within a few wave numbers with the E_u modes already reported in the literature. This may suggest a coexistence of phases in the crystal used by Homes *et al.* The other modes reported in Ref. 1 could, instead, be explained in terms of local vibrations. These latters are related to local lattice distortions produced by the carriers in polar compounds, and their frequencies may differ by tens of wave numbers from those of the extended phonons. Such absorption lines have indeed been observed in metallic NCCO (Ref. 7) and in other cuprates at low T,[8] superimposed to the Drude contribution.

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