Comment on "Mechanism for Electric Field Effects Observed in $YBa_2Cu_3O_{7-x}$ Films"

In a recent Letter [1], experiments with applied electric fields on YBaCuO films are explained in terms of the effect of the interaction between the local field seen by the basal-plane O ions $\mathbf{E}_{\rm loc}$ and their permanent electric dipole moments $\mathbf{p}_i$, on the O ordering assumed governed by the asymmetric next-nearest-neighbor Ising (ASYNNNI) model.

I would like to point out that this explanation is unlikely for the following reasons:

(1) The authors, using the Lorentz relation (actually valid for a cubic environment) $\mathbf{E}_{\rm loc} = (2 + \epsilon)\mathbf{E}_m/3$ and a very large dielectric constant $\epsilon \sim 400$ point out that the local field is ~130 times larger than the macroscopic field $\mathbf{E}_m$, and assume $\mathbf{E}_m$ of the order of a potential drop of 10 eV over a 100 Å film. However, if $\epsilon \sim 400$, in the experiment [2], most of the potential drop takes place in the 5000 Å thick $SrTiO_3$ substrate. Taking a dielectric constant ~1000 for $SrTiO_3$ at 100 K [3], a simple calculation gives $\mathbf{E}_m \sim 5 \times 10^{-3}$ V/Å. Thus, the interaction $-\mathbf{E}_{\rm loc} \cdot \mathbf{p}_i$ is too small to affect the O ordering.

(2) If $\mathbf{E}_{\rm loc}$ were indeed of the order of 13 V/Å, the induced O moments $\mathbf{p}_{\rm ind}$ would be much larger than the permanent ones. Using the linear relation $\mathbf{p}_{\rm ind} = \alpha \mathbf{E}_{\rm loc}$ (although not valid for such a huge electric field), $\mathbf{p}_{\rm ind} \sim 3e$ Å is obtained [4]. Moreover, a field of this order of magnitude should have dramatic consequences on the conductivity (electric breakdown [5]).

(3) The analysis of the resistivity is based on Eq. (3) of Ref. [1], which assumes that fourfold and threefold coordinated Cu ions have charge +2 while twofold coordinated ones are Cu^+. This might be a reasonable hypothesis in the ionic limit, but is incorrect when covalency is taken into account [6]. A quantitative estimate of the number of holes in the superconducting planes can be given only by a many-body calculation of the electronic structure.

(4) On general physical grounds one expects that the number of threefold coordinated ions given by the ASYNNNI varies exponentially with V_2/T. A recent calculation gives $n_3 \sim \exp(2V_2/T)$ [7]. Thus, for $T =$ 100 K $n_3 \sim 6 \times 10^{-4}$, and according to Ref. [7] $n_3 =$ 0.015 at 200 K. This means that the ASYNNNI predicts an almost perfectly ordered structure at low temperature and no decrease of the resistivity as a consequence of O reordering is possible, unless one starts from a metastable state. This state, however, implies low mobility of the O ions and a dependence on the preparation method which contradict the authors' hypothesis. In addition, the resulting exponential temperature dependence of the hole concentration contradicts experiment.

(5) It is very unlikely that a photon of energy 1.9 eV displaces an O atom. In an elastic collision, the maximum speed that the latter can gain is $v \sim 8$ cm/s and the maximum possible O displacement is of the order of v times an average of the inverse of the O phonon frequency, i.e., less than 10^{-4} Å. The observed persistent photoconductivity [8,9] is most noticeable for oxygen lean samples, near the insulator-metal transition. For these samples there is experimental [10] and theoretical [6,11] evidence that $V_2 > 0$ and the system does not order in "chain" structures (CS) but in nearly "hexagonal" structures (HS) with regularly spaced O atoms. A possible interpretation of the experiments is that illumination promotes carriers to the superconducting CuO_2 planes, lowering at the same time the resistivity and the screening length. The latter fact destabilizes the HS and the O atoms tend to form chains [6]. When illumination ceases, the O atoms build again the HS, which is stable and semiconducting. Note that if the stable structure were a CS, the increase of the resistivity after ceasing the illumination could not be explained. Well inside the metallic phase, the effect can be explained in terms of CS but with a significant n_3 which is reduced by illumination [9]. This requires either positive or small V_2, in agreement with Refs. [6,11].

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