Interrelation of charge ordering and peculiarities of elastic properties of HTSC

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In this work from the uniform point of view a detailed analysis of anomalous elastic properties of cuprate superconductors (as polycrystal and single crystal samples) is given. It is shown that the abnormal temperature behavior of elastic properties is strongly anisotropic and apparently connected to the formation of charge ordering.

Already the first investigations of high temperature superconductors have revealed a variety of essential features in the temperature dependencies of velocity (v(T)) and attenuation (α(T)) of ultrasound. So for the best investigated isostructural series of HTSC compounds (RE)$Ba_2Cu_3O_{7-\delta}$ (RE - rare earth atom) in the temperatures region 190 - 230 K step changes of v(T) have been observed, indicating on lattice instabilities and/or phase transitions at temperatures previous to the superconducting transition A distinct thermal hysteresis was observed between 60 and 230 K [1]. Further investigations have shown that the hysteretic behavior of v(T) is observed for all isostructural series (RE)$Ba_2Cu_3O_{7-\delta}$, (RE)$Ba_2Cu_3O_8$ and also for the Bi, Pb, Tl HTSC compounds. The hysteretic behavior of v(T) recently was observed by us and in $Ba_xK_{1-x}BiO_3$ compound [2]. The huge temperature hysteresis of velocity of sound and internal friction was observed also in $La_{0,8}Sr_{0,2}MnO_3$ single crystals [3]. For $Ba_xK_{1-x}BiO_3$ and (RE)$Ba_2Cu_3O_8$ compounds the hysteretic behavior of ultrasound can not be closely related to redistribution of oxygen atoms or twinning.

Our theoretical analysis of temperature dependencies of sample resonant frequencies and ultrasonic wave velocity as in YBa2Cu3O$_{7-\delta}$ single crystal samples with various twinning structures and in polycrystal samples measured over a broad range of frequencies (100 kHz ÷ 20 MHz), shows strong anisotropy of hysteretic behavior of elastic moduli. Namely, the C_{3333} and in much smaller degree C_{2323} moduli have hysteretic temperature dependence. While the moduli C_{1111}, C_{2222}, C_{1212} and C_{1313} do not show abnormal temperature dependence.

The fact of existence of strong anisotropy of hysteretic behavior of elastic modulus is important from the point of view of clearing up of the microscopic mechanism of so unusual behavior. Really, the essential contribution to anisotropy of a tensor of elastic modulus is given by interactions of atoms of the nearest coordination spheres of a crystal. Having expressed the tensor of elastic moduli as a function of the constants of pair interactions of atoms in YBa2Cu3O$_{7-\delta}$ crystal it can be shown that the abnormal temperature behavior of the elastic modulus C_{3333} is caused by change with temperature of force constants of the apical oxygen atoms. In used approach the modulus C_{3333} is determined by the interaction of apex oxygen atoms with copper and barium atoms but as abnormal temperature behavior of the elastic moduli C_{1111}, C_{2222} is not observed, a sole opportunity is temperature renormalization of the O(4) oxygen - copper force constants. The given conclusion is consistent with experimental results in which the features in dynamics of O (4), O(1) oxygen atoms in YBa2Cu3O$_{7-\delta}$ were observed also. From the point of view of study of dynamics of atoms in YBa2Cu3O$_{7-\delta}$ the recently published article [4] is of interest. In [4] it is shown that in the temperature region 100 - 200 K incoherent lattice fluctuations essentially surpass thermal ones. Growth of incoherent lattice fluctuations $u(T)$ were observed at temperature $T < T^*_1 = 200K$ and the critical temperature T^*_1 is attributed in [4] to the formation of charge ordering. It is very interesting that the temperature interval in which incoherent lattice fluctuations exceeds thermal coincides with the interval in which hysteretic behavior of speed of ultrasound is observed. And the temperature of formation of charge ordering T^*_1 corresponds to the temperature of opening of a hysteresis loop. In this connection I shall pay attention to the experimental result [5] where hysteretic behavior of ultrasonic wave velocity in CuO crystals was observed. And recently in this compound charge-ordered domains were revealed [6]. Charge-ordered domains with necessity results in occurrence of correlated states of lattice degrees of freedom and may be the reason of formation in a crystal of strongly correlated groups of atoms. Being grounded on the offered by us model of strongly correlated sublattice for an explanation of hysteretic behavior of ultrasonic wave velocity and thermal conductivity in YBa2Cu3O$_{7-\delta}$ crystals [7] the temperature dependence $u(T)$ have been calculated. The calculated curve $u(T)$ describes experimental results for temperatures $T < T^*_1$ (see Fig.1). However at higher temperatures on the experimental dependence $u(T)$ essential growth of incoherent lattice fluctuations is observed. The given growth of fluctuations may be caused by a disordering of oxygen atoms in the Cu(1)-O(1) chains. Really, a quiet large anomaly of a linear expansion coefficient was observed in nearly optimally doped (δ=0.68) of YBa2Cu3O$_{7-\delta}$ untwined single crystals in the same temperature region [8]. But in fully oxygenated (δ=7.0) crystals such anomaly were absent (see inset in fig. 1). I have revaluated the $u(T)$ temperature dependence with taking into account a disordering of vacancies of atoms of oxygen (Fig. 1, curve 3). One can see that the calculated temperature dependence well enough describes the experimental results. Thus, the analysis performed shows that observed ex-

perimentally incoherent lattice fluctuations in $YBa_2Cu_3O_{7-\delta}$ crystals is caused by particular dynamics of oxygen atoms and the hysteretic behavior of the C_{3333} elastic modulus may be attributed to the formation of charge ordering at temperatures $T < T^*_1$.

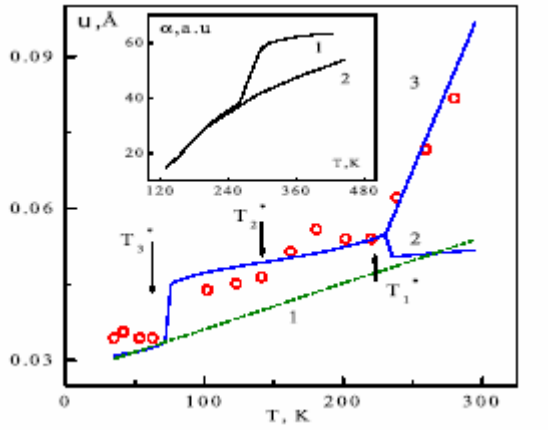

Fig. 1. Temperature dependence of incoherent lattice fluctuation in $YBa_2Cu_3O_{7-\delta}$ crystals. Points are experimental results [4]. Lines are calculated temperature dependencies: 1 - Debye model; 2,3 - model of strongly correlated sublattice without and with taking into account disordering of oxygen atoms in Cu(1)-O(1) chains. On the inset - expansivity versus temperature of untwined $YBa_2Cu_3O_{7-\delta}$ single crystals for δ= 6:95 (curve 1) and δ= 7(curve 2) [8].

This work was partly supported by INTAS organization under grant No. 01-0278.

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