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Lattice Dynamics of Superconducting Metals Y, Zr and Mo

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ABSTRACT: Superconductors include mercury and some other elements such as lead, indium, and tin. They are perfect superconductors in that they have zero resistance below T_c and repel magnetic fields. Their critical temperatures are low, reaching only 7 K for lead.

KEYWORDS-superconductors,lattice,dynamics,metals,magnetic,fields

I. INTRODUCTION

Superconductivity is a set of physical properties observed in certain materials where electrical resistance vanishes and magnetic fields are expelled from the material. Any material exhibiting these properties is a **superconductor**. Unlike an ordinary metallic conductor, whose resistance decreases gradually as its temperature is lowered, even down to near absolute zero, a superconductor has a characteristic critical temperature below which the resistance drops abruptly to zero.^{[1] [2]} An electric current through a loop of superconducting wire can persist indefinitely with no power source.^{[3][4][5][6]}

The superconductivity phenomenon was discovered in 1911 by Dutch physicist Heike Kamerlingh Onnes. Like ferromagnetism and atomic spectral lines, superconductivity is a phenomenon which can only be explained by quantum mechanics. It is characterized by the Meissner effect, the complete cancellation of the magnetic field in the interior of the superconductor during its transitions into the superconducting state. The occurrence of the Meissner effect indicates that superconductivity cannot be understood simply as the idealization of perfect conductivity in classical physics.

In 1986, it was discovered that some cuprate-perovskite ceramic materials have a critical temperature above 90 K ($-183\text{ }^\circ\text{C}$).^[7] Such a high transition temperature is theoretically impossible for a conventional superconductor, leading the materials to be termed high-temperature superconductors. The cheaply available coolant liquid nitrogen boils at 77 K ($-196\text{ }^\circ\text{C}$) and thus the existence of superconductivity at higher temperatures than this facilitates many experiments and applications that are less practical at lower temperatures.

The phonon density-of-states of transition metal diborides TM_2B_2 with $\text{TM} = \text{Ti}, \text{V}, \text{Ta}, \text{Nb}$ and Y has been measured using the technique of inelastic neutron scattering. The experimental data are compared with ab initio density functional calculations whereby an excellent agreement is registered. The calculations thus can be used to obtain electron-phonon spectral functions within the isotropic limit. A comparison to similar data for MgB_2 and AlB_2 which were subject of prior publications as well as parameters important for the superconducting properties .

Even after the first conceptions^{2,3} had provided adequate explanations for this phenomenon, the discoveries⁴ of unanticipated superconducting states in cuprates have raised further questions and, hence, induced massive

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explorative efforts. To account for the findings of superconductivity in cuprates, considerable attention was paid to the influence of electron spectrum instabilities (“singularities”), which are located at the Fermi levels of superconductors.^{5,6} Namely, the aforementioned electron spectrum instabilities are assumed to induce a structural distortion, which is counterbalanced by electrons residing in steep bands (“flat band/steep band scenario”).^{7,8} The latter idea⁷ implies that the occurrence of a superconducting state tends to be linked to the presence of a flat band at the Fermi level in a given material. In this context, one may also consider that a particular composition could affect the position of a flat band relative to the Fermi levels in a given series of isostructural compounds, as atomic substitutions and/or structural defects influence the chemical compositions and, furthermore, the electronic (band) structures within such a set of materials.⁹ Indeed, previous^{10,11} temperature-dependent electric resistance measurements for series of isostructural compounds revealed that metal-to-superconductor transitions are observed solely for those species for which singularities are “pinned” to the Fermi levels. Besides atomic substitutions,^{12,13} structural defects (“vacancies”) also influence the chemical compositions, electronic band structures, and, ultimately, the physical properties of compounds existing over certain homogeneity ranges. For instance, previous research^{14–16} on cuprates forming over certain homogeneity ranges showed that the presence and, furthermore, temperatures of metal-to-superconductor transitions are linked to the amounts of oxygen vacancies in the crystal structures. Another series of superconductors, which form over certain homogeneity ranges, has been identified for chalcogenides crystallizing with the rock salt-type structure.^{17,18} More recent research¹⁹ on the electronic band structures of such rock salt-type chalcogenides based on initial, defect-free structure models revealed that flat bands were located near, but not at the Fermi levels in several of these compounds. In the flat band/steep band scenario,^{7,8} such an outcome suggested an absence of metal-to-superconductor transitions being in stark contrast to the experimentally determined^{17,18} results. This apparent discrepancy was explained by additional investigations showing that the locations of flat bands relative to the Fermi levels ought to be manipulated by the presence of vacancies in the crystal structures of these chalcogenides. But, what are the driving forces to crystallize with compositions that are related to vacancies in the crystal structures of the respective rock salt type chalcogenides? To answer this question, we sought to investigate the electronic as well as vibrational properties, and the nature of bonding for a series of prototypical chalcogenide superconductors, i.e., MS (M = Sc, Y, Zr, Lu).

To provide greater insight into the vibrational properties of the zirconium-containing sulfides, the vibrational properties were also examined for Zr₃S₄, which has been previously reported²⁰ to crystallize with a superstructure of the respective rock salt type sulfide. The compositions of the aforementioned, metal deficient structure models were chosen considering the experimentally determined phase widths of the superconducting sulfides, which have been reported elsewhere.^{17,18} Full structural optimizations, which included lattice parameters and atomic positions, were carried out for all materials using the projector-augmented wave method²¹ as implemented in the Vienna ab initio simulation package^{22–23} (VASP). Correlation and exchange in all computations were described by the generalized gradient approximation of Perdew, Burke, and Ernzerhof, and the energy cutoff of the plane wave basis sets was 500 eV. In the cases of the electronic band structure computations of constituting elements, i.e., Sc, Y, Lu, Zr, and S, sets of up to 16 × 16 × 16 k-points were used, while sets of 16 × 16 × 16 and 8 × 8 × 8 k-points were employed for MS (M = Sc, Y, Zr, Lu) and M₃1S₃2 (M = Sc, Y, Lu), Zr₂9S₃2, and Zr₃S₄, respectively. All computations were considered to have converged as the energy difference between two iterative steps fell below 10^{−8} (and 10^{−6}) eV/cell for the electronic (and ionic) relaxations. The coordinates of the high-symmetry k paths within the Brillouin zones were generated utilizing the AFLOW²⁸ code, and the electronic band structures of all sulfides were visualized with the aid of the Python Materials genomics (pymatgen) program. The vibrational properties of MS (M = Sc, Y, Zr, Lu), M₃1S₃2 (M = Sc, Y, Lu), Zr₂9S₃2, and Zr₃S₄ were examined using the

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Parlinski–Li–Kawazoe³⁰ method as implemented in the Phonopy³¹ code. In this approach, the phonon frequencies are determined based on force constant matrices, after the corresponding sets of the interatomic forces have been computed within supercells, in which a particular atom had been elongated. The interatomic forces were calculated using VASP in the Γ -point approximation, an approach that has largely been employed elsewhere. The supercells employed in the computations corresponded to $4 \times 4 \times 4$ and $2 \times 2 \times 2$ expansions of the structurally optimized unit cells of Zr

II. DISCUSSION

In case of Mo, the properties investigated are the critical magnetic field and associated supercooling, and also the thermal and electrical conductivity in both the superconducting and the normal states. The interest in molybdenum arises from the position it occupies among the transition metals in the periodic table. The study of Mo yields a basis for the comparison of its superconducting properties to those of its neighboring elements and thus provides more insight into the phenomenon of superconductivity in the transition metals. Therefore, before dwelling upon the details of the investigations carried out in this experiment, it seems most pertinent to present first a sketch of the situation in the transition metals and discuss the properties of molybdenum as a member of this group. The superconducting properties of the transition metals have been the subject of many experimental and theoretical investigations in recent years. The new purification techniques have made it possible to discover superconductivity in many of the elements of this group and their alloys, and furthermore, have made available a wealth of experimental observations on their related properties. These observations have revealed marked differences between the superconducting properties of the transition and non-transition metals. Unlike the latter, the transition metals do not seem to obey some of the laws derived from the simple theory of phonon-induced superconductivity of Bardeen, Cooper, and Schrieffer³² (BCS). However, within their group, these elements seem to behave in a regular and symmetric manner³³ for which even empirical laws can be established. Moreover, the variation of the properties from one element to the next, along a series, is rather smooth as can be observed from the study of alloys of these elements with their nearest neighbors. The major distinction between the transition and non-transition metals is the presence of a partially filled d-band in the transition metals. It should also be noted that some of the rare earth elements, too (with partially filled f-bands), have anomalous superconducting properties similar to the transition metals. Therefore, one associates the anomalies in the superconducting properties with the role of the unfilled bands. With this in mind, to explain the superconductivity of the transition metals, one can either look for new mechanisms as the cause of superconductivity or apply the electron-phonon-interaction model by taking into account the details of the energy band of the d-electrons. In the following discussion, we briefly review some of the crucial observations on the transition metals as well as the theoretical models and calculations which have been proposed to explain them. We concentrate on the central transition metals since Mo belongs to this group. We restrict the mentioning of the observations to the case of Mo, and only when necessary, we discuss the experimental results on its neighboring elements.

III. RESULTS

Molybdenum has a bcc crystal structure with the number of conduction electrons per atom, $Z = 6$. Superconductivity in molybdenum was first reported by Geballe et al. Its properties can best be understood by comparison to those of its neighboring elements in the periodic table. Theoretical calculations of the band structure of Mo along with that of W and Cr have been made by Loucks. The Fermi surfaces of Mo and W are found to be identical and different from that of Cr. In fact the role of W in the 5d-series is similar to the role of Mo in the 4d-series. Thus we limit the

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discussion to the comparison of the superconducting properties of Mo with those of its neighboring elements in the 4d-series. It is helpful to study the empirical information relating the band structure and other properties of these metals. The comparison is made as a function of Z . Because of the extensive mutual solubility of the transition metals, one can, by making alloys of neighboring elements, smoothly vary a given property from one element to the next. Therefore, the parameter Z can be considered as a continuous variable. In the present discussion we consider the region $5 \leq Z \leq 7$. In this region, the study of the specific heat constant γ which is a measure of the Fermi surface density of states, shows a minimum at $Z = 6$. A similar minimum is observed in the magnetic susceptibility. The minimum in the density of states at $Z = 6$ for the transition metals has qualitatively been explained in terms of a universal model for the conduction band: a "rigid band structure" into which electrons are "poured" and the properties of a given element depend on its number of conduction electrons. According to the rigid band model, the effective potential seen by an electron of d -symmetry consists of a screened ion interaction, $-z(r)e^{-r}$ and a centrifugal barrier $3\hbar^2/mr^2$ and forms a potential well. If an electron is scattered from such a potential well, it is possible that the scattering cross section shows a sharp peak as a function of energy corresponding to a virtual bound state of energy in the potential well, i.e., a scattering resonance.

IV. CONCLUSION

We show that a second-phase diagram is needed to describe "overdoped" cuprates prepared by high-pressure oxygen methods. The transition temperatures of HPO compounds continue to increase past the values of O stoichiometry and Cu charge where the superconductivity in conventional materials terminates. The Mo and Cu maintain their preferred geometries despite the higher Cu charge via clustering of the Mo. The principal effect of the Mo and excess O is therefore nanophase separation into Mo- and Cu-enriched domains. The high degree of similarity between the HPO and normal structures, including a Cu₂-apical O two-site distribution, therefore suggests that the elevated T_c of YSCO-Mo may originate in a combination of this nanoscale heterogeneity and the dynamical properties. A common characteristic of many "overdoped" cuprates prepared with high-pressure oxygen is T_c values ≥ 50 K that often exceed that of optimally doped parent compounds, despite O stoichiometries that place the materials at the edge or outside of the conventional boundary between superconducting and normal Fermi liquid states. X-ray absorption fine-structure (XAFS) measurements at 52 K on samples of high-pressure oxygen (HPO) YSr₂Cu_{2.75}Mo_{0.25}O_{7.54}, $T_c = 84$ K show that the Mo is in the (VI) valence in an unusually undistorted octahedral geometry with predominantly Mo neighbors that is consistent with its assigned substitution for Cu in the chain sites of the structure. Perturbations of the Cu environments are minimal, although the Cu X-ray absorption near-edge structure (XANES) differs from that in other cuprates. The primary deviation from the crystal structure is therefore nanophase separation into Mo- and Cu-enriched domains. There are, however, indications that the dynamical attributes of the structure are altered relative to YBa₂Cu₃O₇, including a shift of the Cu-apical O two-site distribution from the chain to the plane Cu sites. Another effect that would influence T_c is the possibility of multiple bands at the Fermi surface caused by the presence of the second phase and the lowering of the Fermi level.

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