Strain-induced superconductivity in RuO_2

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Abstract

First-principles calculations were performed on RuO_2 strained along (001) and (100) planes. We find that biaxial tensile strain on the (001) plane lead to an increase in the density of states (DOS) near Fermi level (E_F). Similarly, we study the biaxial strain on the (100) plane and find that tensile strain along the b-axis and compressive strain along the c-axis also increases the DOS near E_F. According to weak coupling theories of superconductivity, increasing DOS near E_F is expected to increase the superconducting transition temperature T_c. We report two candidate direction of strained RuO_2 which could potentially induce superconductivity that was recently observed in RuO_2/TiO_2(110).

I INTRODUCTION

Superconductivity is a phenomenon where materials can achieve zero resistivity below a critical temperature T_c. These materials have rapidly become important in many medical and engineering fields [1].

Weak coupling theories of superconductivity have parameterized T_c as [2]:

$$T_c \sim \omega_B e^{-\frac{1}{N(E_F)V}} = \omega_B e^{-\frac{1+\lambda}{\lambda-\mu^*}},$$

where ω_B refers to the energy scale of bosons that mediate the attraction V between electrons. λ refers to the electron-phonon coupling strength, μ^* is the Coulomb pseudopotential and $N(E_F)$ is the density of states (DOS) at the Fermi Level (E_F). This equation suggests that increasing $N(E_F)$ could increase T_c.

Recently, epitaxial strain engineering was used to induce superconductivity in RuO_2, which became the first example of strain inducing T_c in a metal [3]. RuO_2 grown on TiO_2 substrate on the (110) plane was found to be superconducting at T_c = 2 K. This transition was attributed to changes in the relative occupancies of *d*-orbitals.

In this report, we expand on this work by studying the changes in the band structure and DOS for strained RuO_2(100) and RuO_2(001) in the hopes of finding potential candidates with a higher T_c than the studied RuO_2(110).

II METHODOLOGY

First-principles calculations were performed using QUANTUM ESPRESSO software package [4]. Scalar-relativistic norm conserving pseudopotentials with PBEsol as the exchange correlation functional were used for both Ru and O [5]. The kinetic energy cut-off for Kohn-Sham wave functions was fixed at 160 Ry. The convergence threshold for total energy and forces was 10^{-4} Ry and 10^{-3} Ry/Bohr respectively. The convergence threshold for self-consistency was set to 10^{-10} Ry. A Γ-centered electron-momentum *k*-mesh of 16 x 16 x 24 was used with Methfessel-Paxton smearing of 0.02 Ry in band structure and 0.005 Ry in DOS calculations.

III RESULTS

A. (001) Strain

Experiment agrees well with theory for the bulk structure with only a deviation of around 0.6% in the lattice constants as shown in Table 1. Our reproduction of bulk results also matches perfectly with the previous theory.

To simulate growth on the (001) plane, we varied lattice constants a and b in increments of 0.5% while lattice constant c was free to relax. Table 1 shows the results of +2.5% biaxial tensile strain and -2.5% biaxial compressive strain in the a-b plane.

Name	a	b	c
bulk RuO_2-expt	4.492	4.492	3.106
bulk RuO_2-DFT (Theory)	4.464	4.464	3.093
bulk RuO_2-DFT (This work)	4.464	4.464	3.093
$RuO_2(001)(-2.5\%)$ - DFT	4.352	4.352	3.149
$RuO_2(001)(+2.5\%)$ -DFT	4.576	4.576	3.031

Table 1: The effect of (001) strain on the lattice constants (in Å). The bulk lattice constants are included for comparison.

The effect of this strain on the band structure and DOS can be seen in Figure 1. For tensile strain, we find that the flat bands between R and Z move closer to E_F. For compressive strain, we find these bands move further away from E_F. This trend is consistent with [3] where biaxial tensile strain in the a-b plane also leads to an increase in $N(E_F)$ and possibly induces T_c. Therefore, based on band structure and DOS calculations biaxial tensile strain on the a-b plane could make RuO_2(001) a viable candidate for enhancing T_c.

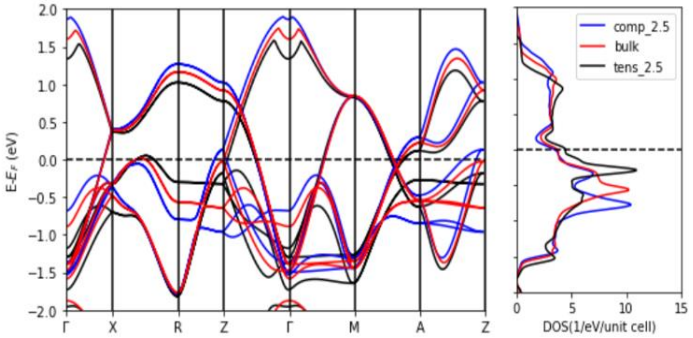

Figure 1: Band structure and DOS of RuO_2 for various (001) strains. The results for unstrained case (red lines), 2.5% compressive strain (blue lines) and 2.5% tensile strain (black lines) in the a-b plane are shown.

B. (100) Strain

To simulate strain on the (100) plane, we constrained the lattice constants b and c while letting lattice constant a relax. The constraint on b and c was such that the original area of the b-c plane was conserved, i.e compressive strain along b while tensile strain along c and vice versa. Table 2 shows the results of the strain on the (100) plane.

Name	a	b	c
bulk RuO2 - expt	4.492	4.492	3.106
bulk RuO2- DFT	4.464	4.464	3.093
RuO2 (100)(b)(-5%)	4.513	4.241	3.256
RuO2 (100)(b)(+5 %)	4.458	4.687	2.946
RuO2 (100)(c)(-5%)	4.461	4.698	2.939
RuO2 (100)(c)(+5 %)	4.510	4.251	3.248

Table 2: Comparison of bulk RuO_2 lattice constants with RuO2(100)(n)(±x%) where n refers to strain along n axis and (±x%) shows the percentage of either compressive or tensile strain along n. (all units of length are in Å.)

Comparing the value of lattice constants in Table 2 we can immediately see that the effect of compressing b is qualitatively similar to applying tensile strain on c and vice versa. This trend is verified by the band structure and DOS plots in Figure 2.

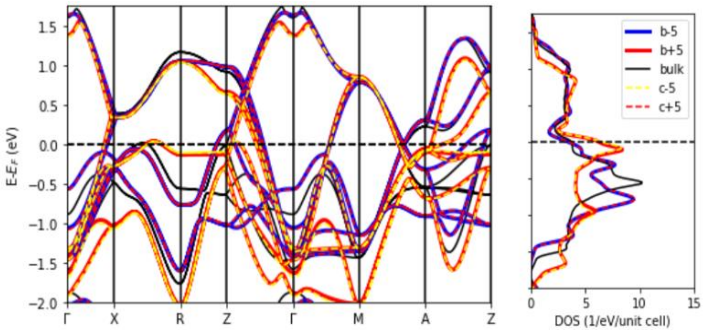

Figure 2: Band structure and DOS of RuO_2 for various (100) strains are shown. Dashed red (yellow) lines for 5% tensile (compressive) strain on c while applying compressive (tensile) strain on b overlaps with the blue (red) line for 5% compressive (tensile) strain on b while applying tensile (compressive) strain on c.

For tensile strain on b and compressive strain on c, we find the flat bands between R and Z move closer to E_F, whereas for compressive strain on b and tensile strain on c, the flat bands move further away from E_F. This trend is consistent with calculations done on (001) strain, where a similar trend was seen. Therefore, based on band structure and DOS calculations, tensile strain on b and compressive strain on c for RuO_2(100) could make it a viable candidate for enhancing T_c.

IV FUTURE WORK

Effects of biaxial strain and uniaxial strain in the RuO_2(110) direction need to be explored. Uniaxial strain along [100] and [001] directions are also yet to be studied. Finally, to calculate T_c, electron-phonon coupling calculations need to be done for each of the respective strains.

V ACKNOWLEDGEMENTS

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