The mechanical and anisotropy properties of α-$RuCl_3$ compound

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ABSTRACT

The recent study showed that the low-temperature crystal structure is described by space group C2/m with lattice parameters a=5.981 Å, b=10.354 Å, c=6.014 Å, and β=108.800. Also, the recent theoretical paper described spin ordered states where FM is ground.
In this study, we have studied the structural, mechanical, and directional dependency of mechanical properties of the α-$RuCl_3$ in monoclinic C2/m structure. The elastic constants of these compounds are calculated, then bulk modulus, shear modulus, Young's modulus, Possion's ratio, Debye temperature, and anisotropy value of polycrystalline aggregates have been derived and relevant mechanical properties are discussed. Furthermore, the directional dependence of the polycrystalline elastic modulus and Poisson's ratio are analyzed from calculated single-crystal elastic constants.

1. INTRODUCTION

The ruthenium chloride ($RuCl_3$) structure has interesting catalytic, photochemical and magnetic properties [1]. A layered honeycomb-lattice compound $RuCl_3$ is considered to be a promising candidate for applying Kitaev spin liquid due to its magnetically properties [2]. Recently, spin states of this compound in monoclinic structure was studied.

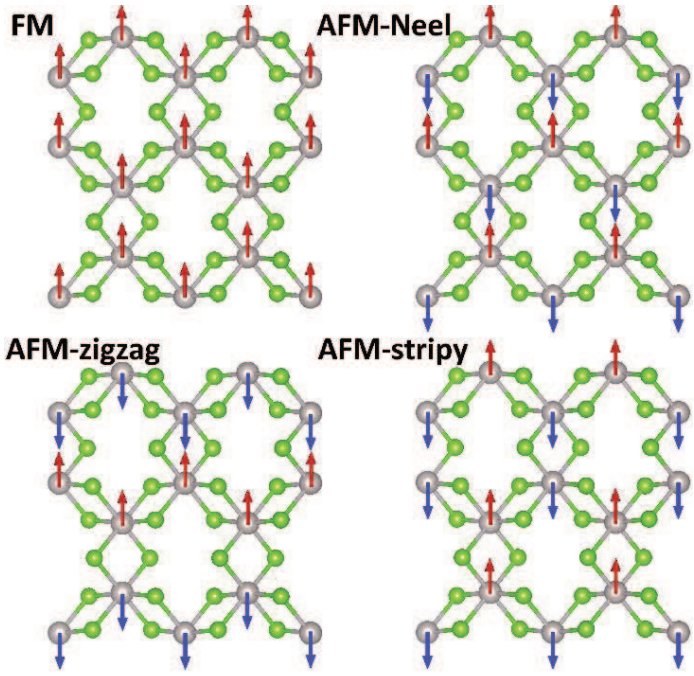

Figure 1. The considered spin-states for monoclinic α-$RuCl_3$ compound.

In this study, the mechanical behavior of $RuCl_3$ are systematically investigated by first-principles within the density functional theory (DFT). The five magnetic state (non-spin, FM, AFM-stripy, AFM-zigzag, and AFM-neel) are considered (See Fig. 1). The method of calculation is given in Section 2, the results and overall conclusions are presented and discussed in Section 3.

2. METHOD

All calculations have been carried by using the VASP code [3-4] based on the density functional theory (DFT). The electron–ion interaction was considered in the form of the projector-augmented-wave (PAW) method with plane wave up to an energy of 400 eV [5], an adequate value for studying the physical properties. The Perdew–Burke–Ernzerhof (PBE) type functional within the generalized gradient approximation (GGA) [6] has been used for the exchange and correlation terms in the electron–electron interaction. 4x8x8 Monkhorstand Pack [7] grid of k-points has been used. The second order elastic constants were predicted by using the stress-strain method implemented in the VASP code [8].

3. RESULTS AND DISCUSSION

3.1. Structural properties

The fully optimized parameters are listed in Table 1 is well agreement with literature data [1]. We found that energetically more favorable state is ferromagnetic (FM).

Table 1. The calculated lattice parameters (a, b, c in Å) and ground state energies (E_0 in eV/fu).

Spin State	*a*	*b*	*c*	E_0	V_0	μ_B	*References*
FM	5.9969	10.424	6.5655	-16.8303	98.357	4	Present
	5.99	10.37	6.05				Exp. [1]
AFM-stripy	6.0758	10.1926	6.5787	-16.8094	97.632	0	Present
AFM-zigzag	5.8596	10.4785	6.5867	-16.8038	97.372	0	Present
Non-Spin	6.1217	9.6956	6.5339	-16.7615	92.855	---	Present
AFM-neel	6.1233	9.7625	6.6495	-16.7782	95.227	0	Present

3.2. Mechanical properties

We have used the "stress-strain" relations [8] to compute the second order elastic constants, and the findings are given in Table 2.

Table 2. The calculated elastic constants (C_{ij} in GPa) for spin states.

Spin State	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}	*References*
FM	44.8	39.9	7.7	1	1.2	9.9	19.5	2.5	2.5	Present
AFM-stripy	53.4	72.8	8	0.9	1.5	25.7	12.7	2.9	2.1	Present
AFM-zigzag	61.1	60.7	7.9	1.1	1.2	19.1	15.8	2.4	2.4	Present
Non-spin	87.6	77.5	10.6	1.2	2.2	27.4	17	4.1	2.9	Present
AFM-neel	62.6	47.9	8.1	1.1	0.4	13.1	14.3	2.5	3	Present

*C_{15}, C_{25}, C_{35} and C_{46} ~0 GPa

All considered states satisfy the stability conditions [9, 10] for α-$RuCl_3$ compound. The mechanical properties, such as bulk modulus (B), Young's modulus (E), shear modulus (G), Poisson's ratio (v), Debye temperature (θ_D in K), the longitudinal, transverse, average elastic wave velocity (v_l, v_t, v_m in m/s) which are functions of the elastic constants, are calculated by using the Voigt–Reuss–Hill approximation [11] and the result are listed in Table 3. Unfortunately, no experimental or other theoretical works exist on these properties for comparison with our results.

Table 3. Calculated bulk modulus (B in GPa), shear modulus (G in GPa), Young's modulus (E in GPa), Poisson's ratio (v), B/G ratio, G/B ratio, Debye temperature (θ_D in K), The longitudinal, transverse, average elastic wave velocity (v_l, v_t, v_m in m/s) for α-$RuCl_3$

	B	*G*	*E*	*v*	*G/B*	*B/G*	θ_D	v_l	v_t	v_m
FM	11.3	4.6	12.1	0.32	0.41	2.46	131.4	2232	1146	1284
AFM-stripy	13	7.9	19.6	0.25	0.6	1.65	169.6	2552	1476	1639
AFM-zigzag	13.1	7	17.8	0.27	0.53	1.87	160.8	2521	1408	1567
nospin	17.2	9.8	24.6	0.26	0.57	1.76	188.1	2856	1622	1803
AFM-neel	12.5	5.4	14	0.31	0.43	2.3	142.3	2360	1239	1385

Bulk modulus, Shear modulus (G), Poisson's ratio (v), Young's modulus (E) which are the most interesting elastic properties for applications, are often measured for polycrystalline materials when investigating their hardness. The results show that α-$RuCl_3$ have soft nature. The typical value of Poisson's ratio is about $v = 0.1$ for covalent materials and 0.25 for ionic materials. In the present values of v is between 0.25-0.32 for the considered spin states. Thus, the ionic contributions to the atomic bonding are dominant for the case. The present values of $G/B \approx 0.6$ strongly support the ionic contribution to inter-atomic bonding.

According to criterion, a material is brittle (ductility) if the B/G ratio is less (high) than 1.75. The calculated value of the B/G (1.65) is less than 1.75 for the AFP-stripy hence, α-$RuCl_3$ will behave in a brittle manner in this state. All calculated Debye temperatures are less than the ambient temperature which shows all modes active in room temperature for α-$RuCl_3$.

4. CONCLUSION

We have performed the first principles total energy calculation for monoclinic α-$RuCl_3$ using the plane-wave pseudopotential approach to the density-functional theory within the generalized gradient approximation. The structural and elastic calculations were done for non-spin, FM, AFM-stripy, AFM-zigzag, and AFM-neel spin states. All considered states satisfy the mechanical stability criteria's and Mechanical behavior does not change between states.

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