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Calculations of structural, elastic and magnetic properties of the novel full Heusler alloys Ru_2XY (X = Nb, Mn) and (Y = Te, Sb)

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Introduction. The interest in Heusler compounds family in the last years has a huge impact on the progress of their applications especially in shape memory effect, magneto-caloric effect, and giant magneto resistance [1–4]. Recently, the structural, electronic, elastic, thermal, and magnetic properties of a number of full Heusler alloys have been studied by many authors [5–9]. In this study we introduce a theoretical investigation on structural, electronic, elastic, and magnetic properties of new full Heusler Ru_2YZ alloys where Y = Mn, Nb and Z = Sb, Te. The pressure effect on the total and partial magnetic moments is included in this study. Among other studies of Heusler alloys, it is worth mentioning [10] which considered the stability of intermetallic Heusler alloys containing transitions metals. Recently pressure effect on different properties of full Heusler alloys have been considered in [9]. The full Heusler X_2YZ compounds have two possible crystals structures. The first one is the Cu_2MnAl structure with the space group Fm3m: #,216 and the other crystal structure is of the Hg_2CuTi-type with the space group F_43: # 225. The theoretical values of the equilibrium lattice constant, magnetic moment, bulk modulus, and its pressure derivative are calculated using the full-potential non-orthogonal local-orbital minimum-basis method (FPLO) using the GGA approximation. The modified Birch–Murnaghan equation of state was used in investigation of the bulk modulus and its pressure derivative. To investigate some elastic properties as shear modulus, Young modulus, and Poisson ratio we have used WIEN2k electronic code.

Result and discussions. We have performed our calculations for both Cu_2MnAl and Hg_2CuTi structures and found that the Cu_2MnAl structure is the most stable structure for these compounds. Our data shows a good agreement with a theoretical study by I. Asfour [8], who has predicted that Cu_2MnAl structure is the stable for these alloys. The magnetic state is the preferred one in these compounds. We have calculated the lattice constant of Ru_2MnSb 6.25 Å, which shows a good agreement with theoretical and experimental data. The total magnetic moment of Ru_2MnSb is 4.017 μ_B. The calculated spin magnetic moment for Ru_2MnTe compound is high 4.835 μ_B. The magnetic moments of Ru_2NbSb and Ru_2NbTe alloys are 1.745 and 1.147 μ_B respectively. The high magnetic moment of these alloys makes them promising materials for different spintronics applications. We investigated the variation of the normalized unit cell volume (V/V_0) under different hydrostatic pressures. We also calculated the pressure effect on the total and partial moments of Ru_2MnSb compound. In Ru_2MnSb and Ru_2MnTe compounds, the main contribution to the total magnetic moment comes from the Mn-atom. The total magnetic moment of Ru_2NbSb shows strong dependence on pressure. We have calculated the bulk modulus B, shear modulus G, Young modulus Y, anisotropic factor A, shear constant (C^1), Cauchy pressure (C_{11}), Poisson ratio ν, and Pugh's ratio B/G for Ru_2MnZ and Ru_2NbZ (Z = Sb, Te).

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1. C. Salazar Meja, R. Küchler, A. K. Nayak, C. Felser, and M. Nicklas, Appl. Phys. Lett. **110**, 071901 (2017).
2. T. Gottschall, E. Stern-Taulats, L. Mañosa, A. Planes, K. P. Skokov, and O. Gutfleisch, Appl. Phys. Lett. **110**, 223904 (2017).
3. I. D. Rodionov, Yu. S. Koshkid'ko, J. Cwik, A. Quetz, S. Pandey, A. Aryal, I. S. Dubenko, S. Stadler, N. Ali,

I. S. Titov, M. Blinov, M. V. Prudnikova, V. N. Prudnikov, E. Lähderanta, and A. B. Granovskii, JETP Lett. **101**, 385 (2015).
4. S. Y. Yu, Z. H. Liu, G. D. Liu, J. L. Chen, Z. X. Cao, G. H. Wu, B. Zhang, and X. X. Zhang, Appl. Phys. Lett. **89**, 162503 (2006).
5. A. Zitouni, G. Remil, B. Bouadjemi, W. Benstaali, T. Lantri, M. Matougui, M. Houari, Z. Aziz, and S. Bentata, JETP Lett. **112**, 290 (2020).
6. M. G. Kostenko, A. V. Lukoyanov, and E. I. Shreder, JETP Lett. **107**, 126 (2018).
7. S. Benatmane and S. Cherid, JETP Lett. **111**, 694 (2020).
8. I. Asfour and J. J. Supercond, Nov. Magn. **33**, 2837 (2020).
9. S. H. Aly and R. M. Shabara, J. Magn. Magn. Mater **360**, 143 (2014).
10. S. Sanvito, C. Oses, J. Xue, A. Tiwari, M. Zic, T. Archer, P. Tozman, M. Venkatesan, M. Coey, and S. Curtarolo, Sci. Adv. **3**(4), e160224114 (2017).