Pis'ma v ZhETF, vol. 113, iss. 5, pp. 326 – 327 

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

*R. M. Shabara*[+*1)], *B. O. Alsobhi*[+1)]

[+]*Physics Department, Faculty of Science, Taibah University, Al-Madinah al Munawarah, 41411 Saudi Arabia*

[*]*Physics Department, Faculty of Science, Damietta University, 34511 New Damietta, Egypt*

Submitted 4 January 2021
Resubmitted 9 January 2021
Accepted 10 January 2021

DOI: 10.31857/S1234567821050062

**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 $\mu_B$. The calculated spin magnetic moment for $Ru_2MnTe$ compound is high 4.835 $\mu_B$. The magnetic moments of $Ru_2NbSb$ and $Ru_2NbTe$ alloys are 1.745 and 1.147 $\mu_B$ 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 $\nu$, and Pugh's ratio B/G for $Ru_2MnZ$ and $Ru_2NbZ$ (Z = Sb, Te).

Full text of the paper is published in JETP Letters journal. DOI: 10.1134/S0021364021050015

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,

[1)]e-mail: rehamph@hotmail.com; sobhibo@yahoo.com

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).