International Journal of Modern Physics B
Vol. 31 (2017) 1850004 (12 pages)

DOI: 10.1142/S0217979218500042

Theoretical investigation of thermoelectric and elastic properties of intermetallic compounds ScTM (TM = Cu, Ag, Au and Pd)

R. Iqbal[*,†], M. Bilal[*,†,‡], S. Jalali-Asadabadi[§],
H. A. RahnamayeAliabad[¶] and Iftikhar Ahmad[*,†,‡,‖]

[*]*Center for Computational Materials Science, University of Malakand, Chakdara 18800, Pakistan*
[†]*Department of Physics, University of Malakand, Chakdara,18800, Pakistan*
[‡]*Department of Physics, Abbottabad University of Science and Technology, Havelian 22010, Pakistan*
[§]*Department of Physics, Faculty of Sciences, University of Isfahan (UI), Isfahan 81746-73441, Iran*
[¶]*Department of Physics, Hakim Sabzevari University, Sabzevar, Iran*
[‖]*ahma5532@gmail.com*

Received 30 April 2017
Revised 8 July 2017
Accepted 11 July 2017
Published 29 August 2017

In this paper, we explore the structural, electronic, thermoelectric and elastic properties of intermetallic compounds ScTM (TM = Cu, Ag, Au and Pd) using density functional theory. The produced results show high values of Seebeck coefficients and electrical conductivity for these materials. High power factor for these materials at room-temperature shows that these materials may be beneficial for low-temperature thermoelectric devices and alternative energy sources. Furthermore, elastic properties of these compounds are also calculated, which are used to evaluate their mechanical properties. The Cauchy's pressure and B/G ratio figure out that these compounds are ductile in nature. The calculated results also predict that these compounds are stable against deforming force.

Keywords: Thermoelectrics; elastic properties; density of states; DFT; spin-orbit coupling.

PACS numbers: 73.50.Lw, 62.20.-x, 71.20.-b, 31.15.E, 71.70.Ej

[‖]Corresponding author.

1. Introduction

The availability of energy is the main requirement for the everyday life. However, in most processes of utilization of energy especially in heat-related phenomenon, the maximum part of energy is wasted to the environment. Thermoelectric (TE) power generation is currently taking increasing interest as it uses waste heat for useful purposes and to achieve this goal, materials with high values of Seebeck coefficient are required. The high Seebeck coefficient values are commonly obtained in materials with narrow bandgap semiconductors low values of carrier concentration.[1] Like thermoelectric power generation, the thermoelectric cooling is also important. Thermoelectric cooling requires low-temperature materials, however, the literature lacks the study of low-temperature as compared to Thermoelectric (TE) materials of high temperature, and the studies of the metallic TE materials are scanty.[2,3] Lin *et al.*[4] study antiperovskite compound SnC_xCo_3 and investigate the TE properties around 250 K and found maximum value of 0.035 for ZT. Recently, Bilal *et al.*[5] also worked on TE properties of $SnNCa_3$ and showed the relation between Seebeck coefficients and spin–orbit coupling (SC) at room temperature. The authors found that Seebeck coefficient increases significantly with the result of described phenomenon.

The drive of this work is to look for low-temperature TE materials in intermetallic. Therefore, we examine the TE properties of metallic compounds Scandium transition metal (ScTM) (TM = Cu, Ag, Au and Pd). The other aspect of this work is to systematically study the effects of SOC on the electronic and thermoelectric properties of these compounds with $3d$, $4d$ and $5d$ electron states. Thermoelectrics gained attention because it produces electricity from waste heat..[6–10] As TE generators directly convert thermal energy to electrical energy, they do not adversely affect the environment.[11] On the other hand, there are no moving parts in TE generators which avoid noise pollution.

Scandium (Sc) forms intermetallic compounds with transition metals (TMs), (TM = Cu, Ag, Au and Pd). These intermetallic materials crystallize in the cubic CsCl (B2) structure with space group Pm-3m (number: 221).[23] These compounds are also well-known for interesting features of strong electron–electron correlations and spin–orbit coupling effects.[18–22] Interesting work is available in the literature on different physical properties of these materials. Different researchers worked experimentally and theoretically on the structural, electronic, elastic, specific heat and magnetic susceptibilities of ScTM (TM = Ag, Cu, Pd, Rh and Ru) compounds.[24–31] Detailed theoretical studies of the electronic structure and phonon properties of ScTM (TM = Ag, Cu, Pd, Rh, Ru) compounds have been carriedout by Arıkan *et al.*[32] using density functional theory (DFT) within the PBE parametrization of the generalized gradient approximation (PBE-GGA) to investigate different ground state properties such as lattice parameter, bulk modulus and first-order pressure derivative of the bulk modulus. Literature clearly indicates dense electronic states in these materials at the Fermi level which is one of the basic properties that predict the effectiveness of a material in thermoelectricity.

Keeping in view of this important aspect, we investigate TE properties of ScTM (TM = Cu, Ag, Au and Pd) at room-temperature. To the best of our knowledge, this is the first ever attempt made on the TE properties of these materials. As these compounds have d states, the correlation and SOC effects play a key role in the physical properties of these compounds. Sasloglu *et al.*[12] reported that correlation effects decrease but SOC effects increase as one moves from $3d$ to $5d$ period of the periodic table. SOC effect is considered as a weak relativistic correction in Schrödinger's equation in condensed matter outside high-energy physics.[13–16] Hubsch *et al.*[17] reported that $3d$ transition metal-based compounds are strongly correlated electron systems due to their high localization nature. SOC caused nontrivial topological order in transition metal-based compounds[18–22] due to its large effect, especially in the $4d$ and $5d$. The SOC and electron correlation can strongly affect the electronic structures of these compounds.[17] We also calculated the elastic constants of these materials which are further used to calculate mechanical properties such as Young's modulus, Hill shear modulus, anisotropy, Poisson's ratio and Kleinman parameter of these materials. Our calculated independent elastic constants are very close to experimental values.

2. Computational Details

In this paper, first principle calculations are carried out using the full potential linearized augmented plane waves plus local orbitals (FP-LAPW+lo) method as implemented in the WIEN2k code[33] within the domain of DFT.[34] The effects of SOC on structural and electronic properties of these materials are calculated using LDA with Huberd potential.[17,34] The radii of the muffin-tin spheres are considered such that no charge leakage is occurred. In order to get best convergence, few restrictions are imposed such that the basis set is expanded in terms of the plane waves up to $R_{\mathrm{MT}}K_{\max} = 7$,[30,47] where R_{MT} is the smallest atomic radius and $K_{\max}$ is the maximum value of the k-vector. The maximum value of angular momentum $l_{\max} = 10$ is considered inside muffin-tin spheres. The cutoff for the Fourier expansion of the charge density was taken to be $G_{\max} = 12$ Bohr^{-1}.

A k-mesh of 3000 k-points is considered in the irreducible wedge of the brilouin zone (WBZ) with a grid size of $14\times14\times14$ using the Monkhorst and Pack scheme.[35] The estimated electronic structures are further utilized to reckon thermoelectric properties like electrical conductivities and Seebeck coefficients using the BoltzTraP code.[36,37] For TE properties, we used 100,000 k-points in the WBZ. Transport coefficient equation which depends on the rigid band approach can be written as

$$\sigma_{\alpha\beta}(\varepsilon) = \frac{1}{N}\sum_{i,k}\sigma_{\alpha\beta}(i,k)\frac{\delta(\varepsilon-\varepsilon_{i,k})}{\delta(\varepsilon)}, \tag{1}$$

where N expresses strength of k-points and the k-dependent transport tensors can be written as

$$\sigma_{\alpha\beta}(i,\mathbf{k}) = e^2\tau_{i,k}v_\alpha(i,\mathbf{k})v_\beta(i,\mathbf{k}), \tag{2}$$

where $v_\alpha(i, \mathbf{k})$ is the group velocity component and τ is the relaxation time. Seebeck coefficient and electrical conductivity both depend upon temperature, T, and chemical potential, μ, that can be calculated from the tensors of transport distribution integration[36,38]:

$$S_{\alpha\beta}(T,\mu) = \frac{1}{eT\Omega\sigma_{\alpha\beta}(T,\mu)} \int \sigma_{\alpha\beta}(\varepsilon)(\varepsilon-\mu)\left[-\frac{\partial f_0(T,\varepsilon,\mu)}{\partial\varepsilon}\right] d\varepsilon, \tag{3}$$

$$\sigma_{\alpha\beta}(T,\mu) = \frac{1}{\Omega} \int \sigma_{\alpha\beta}(\varepsilon)\left[-\frac{\partial f_0(T,\varepsilon,\mu)}{\partial\varepsilon}\right] d\varepsilon, \tag{4}$$

where α and β are tensor indices while e is electron charge, Ω is volume of the unit cell, μ is the carrier concentration and f_0 is the Fermi–Dirac distribution function. Elastic constants are calculated using the Cubic-elastic software.[39]

3. Results and Discussions

3.1. *Structural properties*

The structural optimizations are performed using experimental[23] lattice constants of the ScTM (TM = Cu, Ag, Au and Pd) compounds. The physical properties of the TM compounds depend on the proper localization of the d-orbital. In $3d$-orbitals, strong Coulomb repulsion exists because of the highly localized nature while there is a small repulsion in the $4d$ and $5d$ because of their slightly delocalized nature.[12] In order to treat such systems, where d-orbitals are participating, we need to optimize the Coulomb repulsion U parameter for each compound. The optimization of U for each compound is carried out by adjusting the calculated lattice constants with the experimental values. The U values for the elements of Cu, Ag, Au and Pd are optimized to be 0.44, 0.59, 0.07 and 0.22 Ry, respectively, while this U value is kept constant for scandium, i.e., $U = 0.15$ Ry. The calculated values of the lattice constants for all the compounds along with other ground state parameters like volume and energy are listed in Table 1. It is obvious from the table that the estimated lattice constants for ScTM (TM = Cu, Ag, Au and Pd) compounds using the LDA+U method are in accordance with the experimental values, whereas other approximations LDA, and LDA+SOC underestimate the lattice constants.

3.2. *Density of states*

Electronic structure plays a key role in defining thermoelectric properties of a material. Dense electronic states are required at Fermi level for good TE performance. Total and partial density of states (DOS) for ScCu in spin-up state without the effect of SOC and with SOC is presented in Fig. 1. The DOS of other materials are approximately similar to the DOS of ScCu. Partial DOS shows that d-states of the material play important role in electronic structure and consequently other properties of the material. It is clear from Fig. 1 that the SOC effects split the d-state of Sc and Cu into dz^2, dxy, dx^2y^2 and $dxz + dyz$ states. After splitting, the

Table 1. Experimental and calculated structural properties like lattice constant (a_0) in unit Å, volume (V_0) in unit a.u.,^{3} ground state energy (E_0) in unit Ry of ScTM (TM = Cu, Ag, Au and Pd) by LDA, LDA+U and LDA+SOC.

Materials	Parameters	LDA	LDA+U	LDA+SOC	Exp.	Others
ScCu	a_0	3.172	3.239	3.169	3.256[a]	
	V_0	215.491	229.329	214.782		
	E_0	−4830.018	−4833.878	−4830.030		
ScAg	a_0	3.345	3.422	3.3137	3.416[a]	3.439[c]
	V_0	252.716	270.459	245.557		
	E_0	−12149.930	−12155.949	−12149.983		
ScAu	a_0	3.324	3.378	3.3136	3.373[a]	
	V_0	247.934	260.116	245.526		
	E_0	−39599.944	−39611.977	−39600.479		
ScPd	a_0	3.238	3.282	3.237	3.283[a]	3.206[b]
	V_0	229.250	238.595	228.869		3.329[c]
	E_0	−11609.813	−11615.770	−11609.852		

[a]Ref. 23; [b]Ref. 31 and [c]Ref. 28.

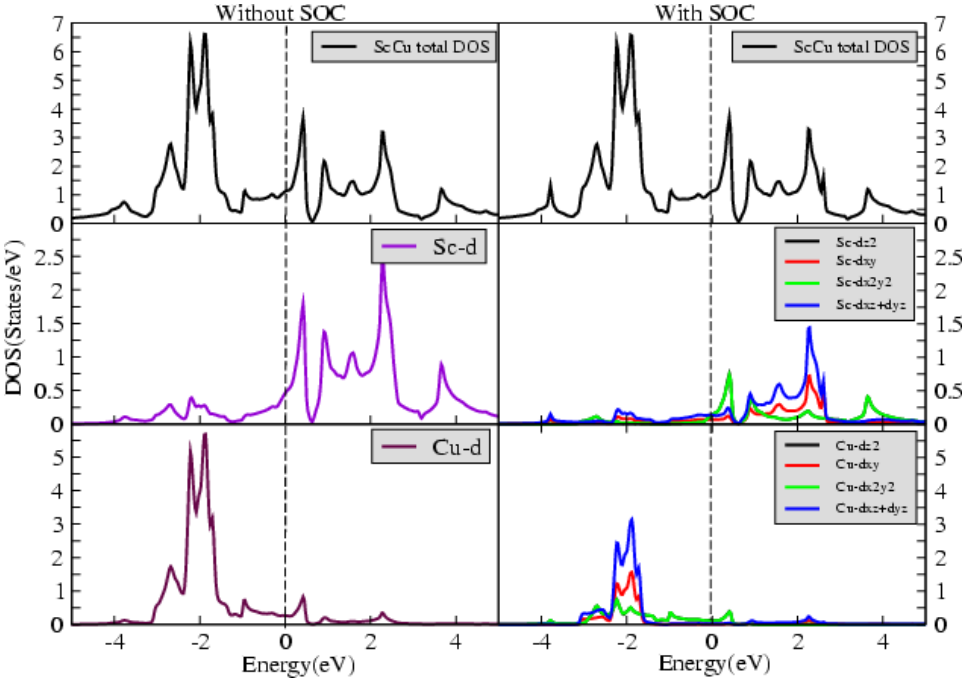

Fig. 1. (Color online) Total and partial DOS for ScCu with and without SOC effects.

combined effect of density of d-states of Sc increases at the Fermi level. Therefore, we can see that DOS at the Fermi level increases due the effect of SOC. This means that SOC effects will consequently enhance the thermoelectric properties of these materials. Other materials also show the same behavior. The figure also shows that the major contributions of the DOS at the Fermi level are due to the d-states of

both elements. The results show that they are metals. The same phenomenon is also observed for the rest of ScTM (TM = Ag, Au and Pd) compounds and similar nature for these compounds are reported in Ref. 32. Apart from this, Fig. 1 also provides information about the dominant contributions of the d-states at the Fermi level in the DOS of ScCu compound that originated from the d sub-states (d_{xy}, d_{x2y2}, $d_{zx} + d_{yz}$) of Sc and (d_{x2y2}) of Cu.

3.3. *Seebeck coefficient*

Seebeck effect is referred to as the potential difference created between two ends of a material as a result of the temperature gradient. Free charge carriers move from hot to cold environment due to the temperature gradient between the ends of a material. For an efficient TE material, we need large values of Seebeck coefficient.

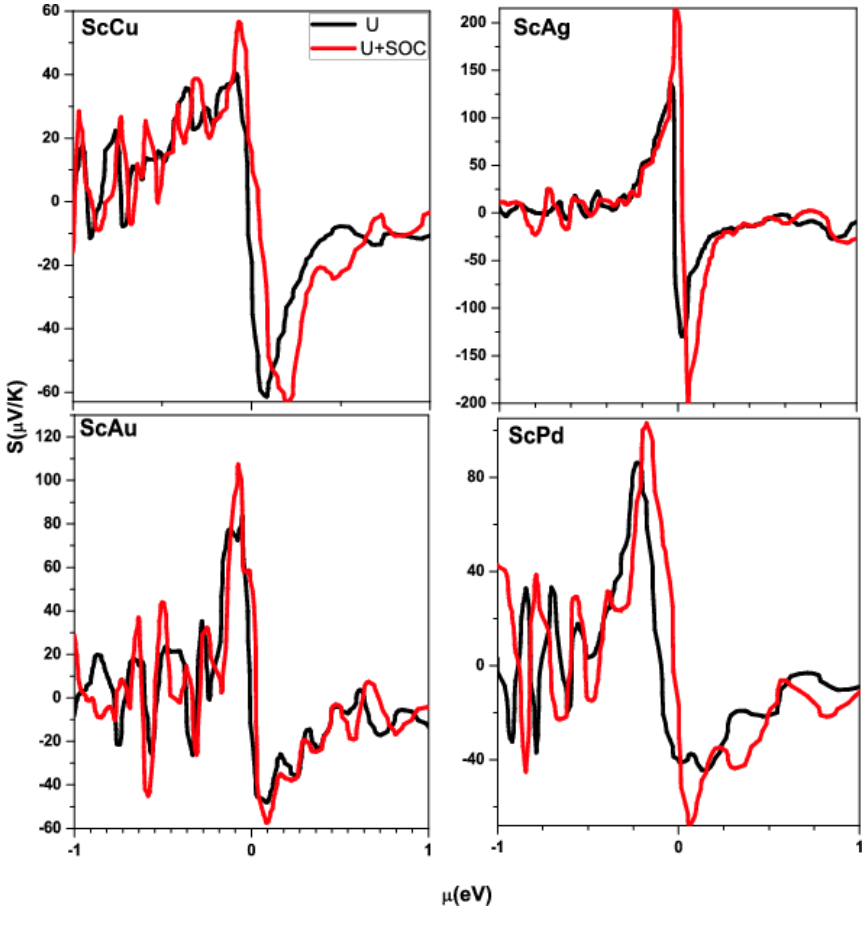

Fig. 2. (Color online) Seebeck coefficients for ScTM (TM = Cu, Ag, Au and Pd) at 300 K temperature as a function of chemical potential with U and U+SOC.

Figure 2 presents the curves of Seebeck coefficients for ScCu, ScAg, ScAu and ScPd at 300 K with and without considering the SOC effects. ScAg shows the highest value of Seebeck coefficient among these materials. All materials show approximately the same behavior with small differences in detail. It is clear from the figure that SOC has a significant effect on the Seebeck coefficient of these materials. SOC effect increases Seebeck coefficients for these materials in both n-type and p-type regions. This is because of the increase in the DOS at the Fermi level by applying SOC effects. For p-type ScAg, Seebeck coefficient reaches the maximum value of 230 μ V/K at -0.05 eV chemical potential. Overall pattern of the Seebeck coefficients of these materials shows that these materials show good response in both n-type and p-type regions. The peak values are obtained between -0.25 and 0.25 eV chemical potential which means these materials will show good thermoelectric properties in this region.

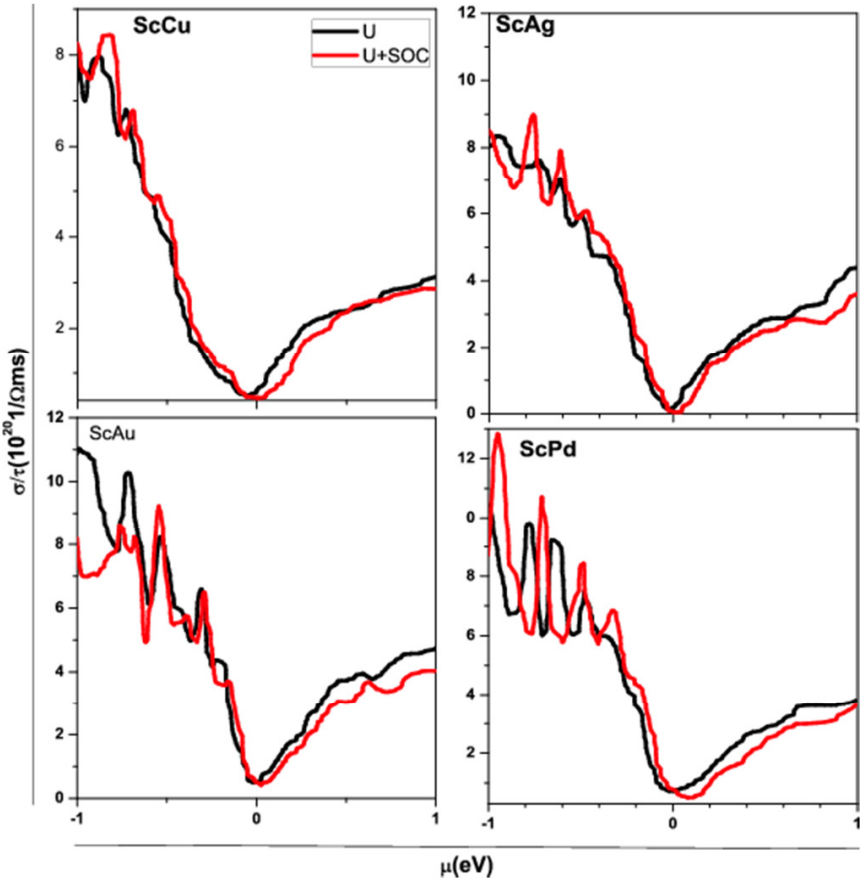

Fig. 3. (Color online) Electrical conductivities for ScTM (TM = Cu, Ag, Au and Pd) compounds at 300 K temperature as a function of chemical potential with U and U+SOC.

3.4. *Electrical conductivity*

Materials with high values of electrical conductivity are required for TE applications. Figure 3 presents electrical conductivities, with and without the effects of SOC for ScTM (TM = Cu, Ag, Au and Pd) compounds against chemical potential at 300 K temperature. The figure shows that electrical conductivities have smallest values near zero chemical potential and increases as chemical potential is increased. For good performance of TE device, we need large values of electrical conductivity. It is clear from the figure that ScAu and ScPd have good TE behavior in the region between −0.25 and 0.25 eV chemical potential as these compounds have nonzero values in this region. In the case of ScAg and ScCu, electrical conductivity stays at zero in the vicinity of −0.25 and 0.25 eV chemical potential. The highest value of electrical conductivity is achieved for ScPd which reaches to approximately $13 \times 10^{20}/\Omega$ ms in p-type region. Furthermore, we can see that all these materials show better response in p-type region compared to the n-type region.

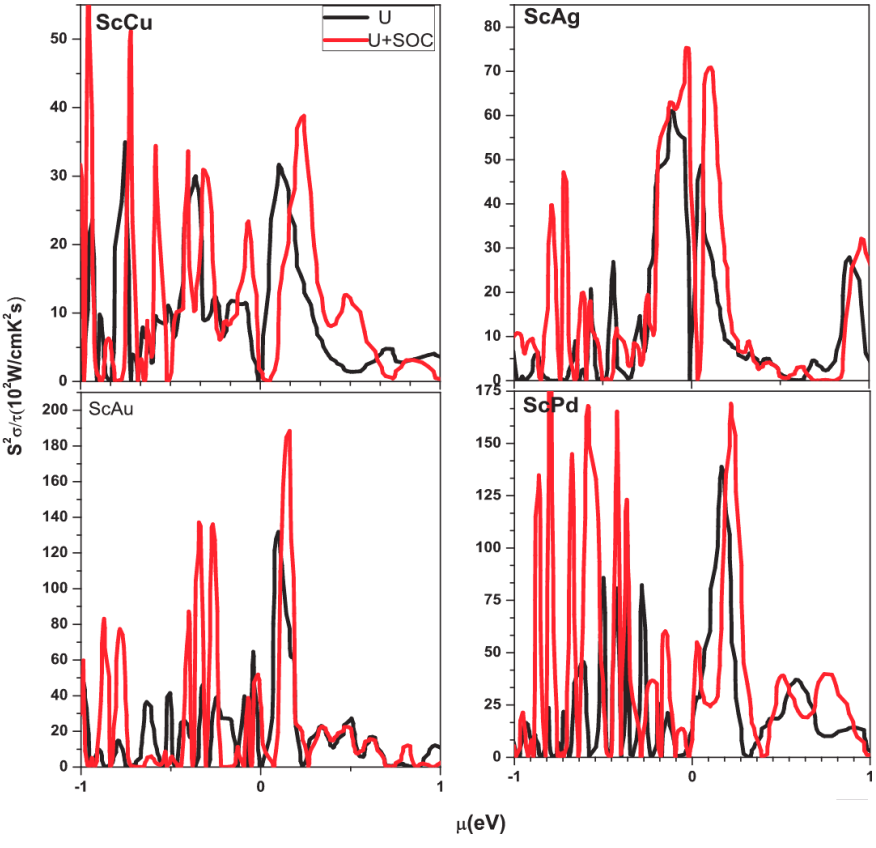

Fig. 4. (Color online) Power factor for ScTM (TM = Cu, Ag, Au and Pd) compounds at 300 K temperature as a function of chemical potential with U and U+SOC.

3.5. *Power factor*

The power factor (PF = $S^2\sigma$) shows the efficiency of a thermoelectric material, where S is the Seebeck coefficient and σ is the electrical conductivity of the material. It is clear from PF that we need large values of Seebeck coefficient and electrical conductivity for better TE performance. Figure 4 presents power factor, with and without the effects of SOC, for ScTM (TM = Cu, Ag, Au and Pd) compounds against chemical potential at 300 K temperature. The figure shows that PF increases with the effects of SOC. ScAu has the highest value of PF among all these materials and with the effects of SOC, it reaches 200×10^2 W/cmK^2 s at 0.2 eV chemical potential at room-temperature. This is because this material has high values of both Seebeck coefficient and electrical conductivity in this region. As the Seebeck coefficient shows good response between -0.25 and 0.25 eV chemical potential, we get the peak values of PF in this region for all materials. Small values of PF beyond this region are due to the large values of electrical conductivity in these regions. Furthermore, we can see that all these materials show a good TE response in n-type as well as in p-type regions.

4. Mechanical Properties

We calculate elastic constants (C_{11}, C_{12} and C_{44}) for ScTM (TM = Cu, Ag, Au and Pd) compounds and compare with the available results. Table 2 shows that all these compounds are mechanically stable under the stability criteria, i.e., $C_{11} - C_{12} > 0$, $C_{11} + 2C_{12} > 0$, $C_{44} > 0$.[42,43] Our results for ScPd are in close agreement with the experimental results.[23] The mechanical properties of these compounds like bulk modulus (B), Young's modulus (Y), shear modulus (G_H), anisotropy (A) and Poison's ratio (ν) are calculated from these elastic constants for each compound.

Shear modulus (G) shows the hardness of a material. The calculated values of shear modulus for the compounds under study are listed in Table 3. It is clear from the table that ScAu has the largest value of shear modulus (52.77 GPa) among all these compounds which shows this compound is the hardest in all these compounds.

Table 2. Calculated values of elastic constants in unit GPa for ScTM (TM = Cu, Ag, Au and Pd) compounds.

Compounds		C_{11}	C_{12}	C_{44}
ScCu	Present	184.370	114.050	64.090
	Other[b]	130.869	70.215	52.425
ScAg	Present	116.900	73.370	62.040
	Other[b]	105.469	68.091	51.307
ScAu	Present	172.630	100.920	68.380
ScPd	Present	169.640	80.650	44.340
	Exp[a]	173.100	106.600	45.500
	Other[b]	151.070	90.850	49.130

[a]Ref. 30 and [b]Ref. 47.

Table 3. The calculated values of Voigt's bulk modulus B, Young's modulus Y, shear modulus G, B/G ratio, Cauchy pressure (C''), Poisson's ratio (v), anisotropy constant (A), Kleinman parameter (ζ) and B/C_{44}.

Comp.	B	Y	G	B/G	C''	ν	A	ζ	B/C_{44}
ScCu	137.48	134.66	50.37	2.73	49.95	0.34	1.8	0.99	2.14
ScAg	87.88	105.97	40.78	2.15	11.33	0.29	2.85	0.99	1.41
ScAu	124.82	138.75	52.77	2.36	32.54	0.31	1.90	0.97	1.82
ScPd	110.3	117.5	44.4	2.48	36.31	0.32	0.99	0.79	2.48

The smallest value of the shear modulus, 40.78 GPa, is for ScAg, which shows that this material has small resistance to deformation.

Young's modulus shows the stiffness of a material.[40] The calculated values of Young's modulus are presented in Table 3. It is clear from the table that ScAu has the largest Young's modulus (138.75 GPa) compared to other compounds hence, ScAu has the highest stiffness among these compounds. The higher values of Young's modulus as compared to the shear modulus exhibit the stiffness of these materials.

The ductile nature of a material is very important from an engineering point of view and can be determined by B/G ratio. For ductile materials, B/G is greater than 1.75 and for brittle behavior of the materials, B/G ratio is lesser than 1.75.[41] Table 3 presents the calculated B/G values for ScTM (TM = Cu, Ag, Au and Pd) compounds. The table shows that all compounds under investigation are ductile. It can be noted from the table that among all ductile compounds, ScPd has the largest value of the B/G ratio (2.48 GPa) and hence reveals a higher value of ductility. Cauchy's pressure ($C'' = C_{12} - C_{44}$) is another parameter to describe the ductile/brittle behavior of a material. The positive value of Cauchy's pressure shows the ductile nature and the negative value indicates the brittle behavior of a material.[42] It is clear from Table 3 that the values of Cauchy's pressure are positive for all these materials which further confirms the ductile nature of all these compounds. The Cauchy's pressure is also used to describe the bonding character in a material..[43] The positive value of Cauchy's pressure corresponds to metallic bonding while the negative Cauchy's pressure attributes to the covalent bond nature. The values of Cauchy's pressure presented in Table 3 indicate that all these compounds have a metallic bond nature.

Poisson's ratio is a very important parameter and may be used to explain various mechanical properties, specifically the incompressibility of a material. The typical value of Poisson's ratio lies between 0 and 0.5. Incompressibility increases as one moves from 0 to 0.5.[44] The calculated values of Poisson's ratio for the compounds are listed in Table 3. It is clear from the table that Poisson's ratios for all these materials fall within the above limit, hence these compounds are low compressible against deformation. Furthermore, this ratio is also used to determine the nature of inter-atomic forces. The typical range of Poisson's ratio for central forces is

0.25–0.5.[45] The calculated values of the Poisson's ratio indicate that dominated inter-atomic forces for these compounds are central forces.

The anisotropy (A) is a parameter, which shows whether the structural properties of a material remain same in all directions or not. For isotropic medium, $A = 1$ and if $A \neq 1$, then the medium will be anisotropic. The calculated anisotropic ratios for all these compounds are listed in Table 3. The table shows that for all these materials, the anisotropic ratio deviates from unity which means their properties vary in different directions; hence, these compounds are anisotropic except ScPd, which has the value approximately equal to one. This shows that this material is nearly isotropic material.

The internal strain of a material is estimated from the Kleinman parameter (ζ). This parameter describes the bond bending and bond stretching. The lower limit ($\zeta = 0$) and upper limit ($\zeta = 1$) correspond to bond bending and bond stretching, respectively. The calculated values of this parameter for the compounds are listed in Table 3. The table shows that in all these compounds, the bond stretching is more dominant than bond bending.

The ratio of bulk modulus to $C_{44}(B/C_{44})$ may be used to estimate the plasticity of a material.[46] Table 3 presents B/C_{44} values for these materials. It is clear from the table that B/C_{44} ratio is highest for ScPd (2.48 GPa) and lowest for ScAg (1.41 GPa). The larger value of B/C_{44} for ScPd (2.48 GPa) indicates the high degree of plasticity.

5. Conclusion

DFT calculations are performed to investigate the structural, electronic, thermoelectric and mechanical properties of ScTM (TM=Cu, Ag, Au and Pd) intermetallic compounds. Our calculated results for structural and elastic properties are in close agreement with the available experimental results. Seebeck coefficient for ScAg gives the highest value of 230 μV/K among these materials. Power factor of 200×10^2 W/cmK^2 is achieved for the ScAu material. The calculated elastic constants obey the mechanical stability criteria suggesting that all these compounds are mechanically stable. The B/G ratio predicted the ductile nature of these compounds. The positive Cauchy's pressure and Poisson's ratio ($v < 0.35$) further confirm the ductility of these compounds. The deviation of anisotropy constant from unity shows the anisotropic nature of these compounds except ScPd whose value is approximately equal to unity. The greater value of B/C_{44} shows the higher degree of plasticity in ScPd compared to other materials.

References

1. M. B. Ricoult *et al.*, US 2014/0225022 A1, 14 (2014).
2. S. V. Ovsyannikov and V. V. Shchennikov, *Chem. Mater.* **22**, 635 (2010).
3. G. D. Mahan, *Solid State Phys.* **51**, 81 (1998).
4. L. P. Tong *et al.*, *Inorg. Chem.* **53**, 3709 (2014).

5. M. Bilal *et al.*, *Mater. Lett.* **11**, 466 (2015).
6. B. Khan *et al.*, *Comput. Physics Commun.* **187**, 1 (2015).
7. H. Ohta, K. Sugiura and K. Koumoto, *Inorg. Chem.* **47**, 8429 (2008).
8. K. Biswas *et al.*, *Nature* **489**, 414 (2012).
9. H. J. Goldsmid and R. W. Douglas, *J. Appl. Phys.* **5**, 386 (1954).
10. T. M. Tritt, *Ann. Rev. Mater. Res.* **41**, 433 (2011).
11. D. S. Dalafave, *Mater. Chem. Phys.* **119**, 195 (2010).
12. E. Sasiogl, C. Friedrich and S. Blugel, *Phys. Rev. B* **83**, 121101(R) (2011).
13. A. L. Marco *et al.*, *Phys. Rev. Lett.* **105**, 216407 (2010).
14. J. Igarashi and T. Nagao, *J. Phys. Soc. Jpn.* **83**, 053709-5 (2014).
15. J. Igarashi and T. Nagao, *Phys. Rev. B* **88**, 104406 (2013).
16. D. Pesin and L. Balents, *Nat. Phys.* **6**, 376 (2010).
17. A. Hubsch *et al.*, *Phys. Rev. Lett.* **96**, 196401 (2006).
18. G. A. Steele *et al.*, *Nat. Commun.* **4**, 1573 (2013).
19. C. Kane and J. Moore, *Phys. World* **24**, 32 (2011).
20. M. Hasan and C. Kane, *Rev. Mod. Phys.* **82**, 3045 (2010).
21. D. Hsieh, *Nature* **452**, 970 (2008).
22. A. Simon *et al.*, *Phys. Rev. Lett.* **102**, 046409 (2009).
23. K. A. Gschneidner Jr. and L. Eyring, *Handbook on the Physics and Chemistry of Rare Earths* (North-Holland Publishing Co., 1979).
24. B. Y. Kotur, *Croat. Chem. Acta* **71**, 635 (1998).
25. B. Perrin *et al.*, *J. Phys. F* **9**, 673 (1979).
26. D. Seipler *et al.*, *J. Phys. F* **7**, 599 (1977).
27. D. Seipler and B. Elschner, *Phys. Lett. A* **55**, 115 (1975).
28. J. Kubler, *J. Phys. F* **8**, 2301 (1978).
29. K. A. Gschneidner Jr. *et al.*, *Acta Mater.* **57**, 5876 (2009).
30. B. Fatima *et al.*, *Intermetallics* **53**, 129 (2014).
31. B. Fatima *et al.*, *Adv. Mater. Res.* **1047**, 27 (2014).
32. N. Arıkan and S. Ugur, *Comput. Mater. Sci.* **47**, 668 (2010).
33. P. Blaha *et al.*, *Phys. Rev. B, Solid State* **12**, 3060 (1975).
34. W. Kohn and L. J. Sham, *Phys. Rev.* **140**, A1133 (1965).
35. H. J. Monkhorst and J. D. Pack, *Phys. Rev. B, Solid State* **13**, 5188 (1976).
36. G. K. H. Madsen and D. J. Singh, *Comput. Phys. Commun.* **175**, 67 (2006).
37. J. Y. Kim *et al.*, *Sci. Rep.* **4**, 5450 (2014).
38. T. J. Scheidemantel *et al.*, *Phys. Rev. B* **68**, 125210 (2003).
39. M. Jamal *et al.*, *Comput. Mater. Sci.* **95**, 592 (2014).
40. C. Jenkins and S. K. Khanna, Mechanics of Materials, *A Modern Integration of Mechanics and Materials in Structural Design* (Academic Press, Cambridge, UK, 2005).
41. P. Wachter, M. Filzmoser and J. Rebizant, *Physica B* **193**, 199 (2001).
42. M. Shafiq *et al.*, *J. Alloys Compd.* **618**, 292 (2015).
43. D. G. Pettifor, *Mater. Sci. Technol.* **8**, 345 (1992).
44. P. H. Mott, J. R. Dorgan and C. M. Roland, *J. Sound Vib.* **312**, 572 (2008).
45. H. Fu *et al.*, *Comput. Matter. Sci.* **44**, 774 (2008).
46. L. Vitos, P. A. Korzhavyi and B. Johansson, *Nat. Mater.* **2**, 25 (2003).
47. M. Rajagopalan and M. Sundareswari, *AIP Conf. Proc.* **1349**, 801 (2011).