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First principles study of the elastic properties of magnesium and iron based bio-resorbable alloys

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ABSTRACT

In the present study, the Density Functional Theory (DFT) implemented in the VASP package has been used to investigate the effects of alloying of different elements deemed biocompatible (Ca, Zn, Li, Zr, Y, Sr, Mn, Ag, RE) when introduced into the Mg and Fe crystal lattice. In particular, the study has been conducted to investigate the general elastic properties, such as bulk modulus, shear modulus, Young's modulus and Poisson's ratio of various Mg- and Fe-based alloys, the results serving to identify candidate bio-resorbable materials potentially suitable for cardiovascular, bronchotracheal, orthopedic and craniofacial applications.

1. Introduction

Bio-inert metals (stainless steels, Ti and Co-Cr-based alloys), biodegradable polymers and bioresorbable ceramics are currently being explored as scaffolds and implants for tissue engineering and regenerative therapies. Metals are more suitable for load-bearing applications due to the combined properties of strength and toughness. However, currently used metallic biomaterials are essentially non-biodegradable, neutral and considered inert *in vivo*, remaining as permanent implants exhibiting no degradable, absorbable or resorption characteristics. As a result, in the case of plates, screws and pins used to secure serious fractures there is inevitably a need for secondary invasive surgical procedure after sufficient healing to remove the implanted fixation devices [1]. Numerous studies (see review [2] and ibid.) have shown the promise of magnesium Mg-alloys as a new class of biodegradable metals for use in stents as well as for craniofacial and orthopedic applications. Magnesium is an exceptionally lightweight metal and has a higher fracture toughness than hitherto used popular ceramic biomaterials such as hydroxyapatite, while its elastic modulus and compressive yield strength are closer to those of natural bone than other commonly used metallic implants.

The desirable low corrosion resistance of Mg, especially in electrolytic and aqueous environments makes it useful for biomaterial applications, wherein the *in vivo* corrosion of the Mg-based implant involves the formation of a soluble, non-toxic hydroxide that is harmlessly excreted in the urine. Magnesium can remain in the body and maintains mechanical integrity over a time scale of 12–18 weeks while the bone tissue heals, eventually being replaced by natural tissue [3].

Magnesium though receiving widespread attention suffers from an undesirable limitation in that pure Mg tends to corrode too rapidly in the physiological system especially with high chloride content releasing hydrogen gas that can cause tissue necrosis and apoptic response in cells. To mitigate this problem various approaches (experimental and theoretical) have been utilized to stabilize the corrosion reaction of the Mg-alloys and also control the eventual release of hydrogen [4–7].

Iron-based alloys are an alternative to Mg-based bio-resorbable alloys if they demonstrate increased corrosion rate compared to pure iron or other industrially used Fe-based alloys when exposed to physiological fluid conditions. These iron based alloys known to date, tend to degrade too slowly, and thus, several studies have been focused on increasing the degradation rates. An iron-manganese binary composition was initially introduced as a biodegradable Fe-based alloy with enhanced corrosion rate and reduced ferromagnetic properties [8]. However, recent literature reports suggest that achieving higher degradation rates in the Fe-Mn alloy system still remains a major challenge and indeed poses a primary limitation preventing the development of biodegradable Fe based alloys for medical device applications [9,10]. For example, in the study [10] elements that are known to exhibit higher aqueous corrosion such as Ca and Mg, well-known for their reactivity in aqueous environments were correspondingly introduced into Fe-Mn alloys to induce higher corrosion of these alloys. As a result, scaffolds of these alloys fabricated using conventional as well as 3-D

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printing approaches result in faster degradation compared to the Fe-Mn matrix as convincingly demonstrated by D. Hong et al. [10].

Although, a large amount of different prospective bio-resorbable Mg- and Fe-based alloys demonstrating appropriate corrosion behavior for bio-applications have been suggested, an aspect that requires keen attention is the influence of the various alloying elements on specific mechanical properties particularly, modulus, strength and ductility. Theoretical determination and experimental validation of the elastic moduli, Poisson's ratio and ductility characteristics will bode to be extremely useful especially when designing these alloys for *in vitro* and *in vivo* experimental studies. Knowledge of such mechanical properties are very important for the bio-resorbable materials in general, and for cardiovascular as well as bronchotracheal stent applications in particular, since the materials being embedded into the blood vessel must be resilient to the several expansion–contraction cycles arising from the blood flow and air flow related pressures subjected to the stent during the lifetime of the implanted stent device. There is therefore, clearly a need for bioresorbable alloys exhibiting high ductility. Consequently, the search for effective alloying elements to improve the ductility of the Mg- and Fe-based alloys will be extremely useful and is strongly encouraged. For these purposes *ab initio* theoretical approaches will be very useful since they obviate the need for expensive and time consuming trial-and-error experimental procedures involving fabrication of alloys combined with tedious mechanical property measurements of several samples being conducted to obtain statistically meaningful and relevant data before implementation in actual *in vivo* applications.

Based on previously reported theoretical and experimental studies [4–7], a list of select binary and ternary Mg- and Fe-alloys has been created and is shown in Table 1. Bulk (B), shear (G), Young's (E) moduli and Poisson ratio (ν) together with B/G ratio qualitatively reflecting the ductility of the materials (see, for example, S. Pugh [11]) have also been summarized in Table 1. All the Mg-based alloys selected are random solid solutions with hexagonal close packed structure, while the Fe-based alloys adopt cubic symmetry of the crystal lattice.

2. Computational methodology and details

In the present study all the elastic constants were determined from the calculated stresses σ_{ij} associated with strains ε_{kl} applied to hydrostatically equilibrated supercells. Using the stress-strain method where the crystal lattice undertakes a series of different normal and shear deformations determined from a relation between the lattice vectors before and after the transformation, such as $Q' = Q(\varepsilon_{kl})$, one can obtain the respective elastic stiffnesses C_{ijkl} based on the calculated stresses σ_{ij} resulting from such deformations and the corresponding Hook's law $\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$.

Five independent elastic stiffnesses should be calculated for the *hcp* crystal structure: c_{11}, c_{12}, c_{13}, c_{33}, and c_{44}, while only three independent stiffnesses c_{11}, c_{12}, and c_{44} will be calculated for the cubic lattice.

Since, in practice all measurements are obtained for polycrystalline materials, the shear modulus G could be approximately estimated from the elastic constants of the single crystals through the Voigt's approximations for maximum values of the moduli:

$$G = (C_{11} - C_{12} + 3C_{44})/5$$

Considering that the bulk modulus, B is identical for single- and poly-crystalline systems given by:

$$B = (C_{11} + 2C_{12})/3;$$

we can further evaluate the polycrystalline-averaged Young's modulus E and Poisson's ratio ν as follows:

$$E = 9BG/(G + 3B);$$

$$\nu = (3B - 2G)/[2(3B + G)] = (3B - E)/6B;$$

wherein

$$C_{11} = (2c_{11} + c_{33})/3$$
$$C_{12} = (c_{12} + 2c_{13})/3$$
$$C_{44} = (2c_{44} + [c_{11} - c_{12}]/2)/3$$

In the present study for calculation of stresses, the Vienna *Ab-initio*

Table 1
Calculated elastic stiffnesses c_{ij} and different moduli for Mg- and Fe-based alloys (in GPa). Experimental data for Mg in parenthesis are from [16].

Alloy	c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	C_{11}	C_{12}	C_{44}	B *Bulk*	G *Shear*	E *Young's*	ν *Poison's ratio*	B/G
Mg	62.4 (59.5)	23.5 (25.9)	22.0 (21.8)	58.9 (61.6)	16.3 (16.4)	61.2 (60.2)	22.5 (23.2)	17.3 (16.5)	35.4 (35.6)	18.1 (17.3)	46.5 (44.7)	0.28 (0.29)	1.96 (2.06)
Mg-$Zn_{0.03}$	50.9	27.1	25.4	56.2	13.5	52.7	26.0	13.0	34.9	13.1	35.0	0.33	2.66
Mg-$Ca_{0.03}$	54.8	31.1	24.0	65.5	16.4	58.4	26.4	14.9	37.1	15.4	40.6	0.32	2.41
Mg-$Ag_{0.03}$	52.6	29.3	22.7	62.8	16.5	56.0	24.9	14.9	35.3	15.2	39.9	0.31	2.33
Mg-$Sr_{0.03}$	59.1	28.5	24.1	66.0	16.8	61.4	25.6	16.3	37.5	16.9	44.1	0.31	2.22
Mg-$Zr_{0.03}$	59.5	27.8	22.8	65.2	19.5	61.4	24.5	18.3	36.8	18.4	47.3	0.29	2.0
Mg-$Y_{0.03}$	62.3	27.0	24.9	68.4	21.5	64.3	25.6	20.2	38.5	19.9	50.9	0.28	1.93
Mg-$Ca_{0.03}Zn_{0.03}$	52.4	28.2	24.6	63.5	16.0	56.1	25.8	14.7	35.9	14.9	39.3	0.32	2.41
Mg-$Ca_{0.03}Zn_{0.03}Zr_{0.03}$	56.7	29.4	23.1	64.5	17.9	59.3	25.2	16.5	36.6	16.7	43.5	0.30	2.20
Mg-$Ca_{0.03}Zn_{0.03}Y_{0.03}$	58.2	28.8	23.1	69.0	20.8	61.8	25.0	18.8	37.3	18.6	47.8	0.29	2.0
Mg-$Ca_{0.03}Zn_{0.03}Sr_{0.03}$	57.6	29.5	23.8	54.0	16.5	56.4	25.7	15.7	35.9	15.5	40.9	0.31	2.31
Mg-$Ca_{0.03}Zr_{0.03}Sr_{0.03}$	58.3	27.4	23.3	57.7	19.1	58.1	24.7	17.9	35.8	17.4	44.9	0.29	2.06
Mg-$Zn_{0.03}Zr_{0.03}Sr_{0.03}$	55.9	23.3	23.6	58.6	17.9	56.8	23.5	17.4	34.6	17.1	44.0	0.29	2.02
Mg-$Zn_{0.03}Y_{0.03}$	56.4	27.5	24.8	66.3	17.7	59.7	25.3	16.6	37.0	16.8	43.8	0.30	2.20
Mg-$Zn_{0.03}Ce_{0.03}$	56.2	27.2	25.0	65.9	18.0	59.4	25.9	16.7	37.0	16.7	43.5	0.30	2.22
Mg-$Zn_{0.03}Nd_{0.03}$	55.9	26.8	24.3	66.4	17.6	59.4	25.1	16.6	36.5	16.8	43.7	0.30	2.17
Mg-$Zn_{0.03}Sm_{0.03}$	56.3	27.1	24.7	65.6	17.5	59.4	25.5	16.5	36.8	16.7	43.5	0.30	2.20
Mg-$Li_{0.03}$ (0.8 wt%Li)	57.4 (59.0)	26.2 (25.9)	24.1 (21.7)	58.6 (61.0)	18.9 (16.2)	57.8 (59.7)	24.8 (23.1)	17.8 (16.3)	35.8 (35.3)	17.3 (17.1)	44.7 (44.2)	0.29 (0.29)	2.07 (2.06)
Mg-$Li_{0.08}$ (2.5 wt%Li)	55.2 (57.9)	27.7 (25.3)	25.7 (21.2)	55.8 (59.7)	20.6 (15.8)	55.4 (58.5)	26.4 (22.6)	18.3 (16.0)	36.1 (34.6)	16.8 (16.8)	43.6 (43.4)	0.30 (0.29)	2.15 (2.06)
Mg-$Li_{0.17}$ (5.4 wt%Li)	54.1	27.4	26.0	54.4	17.9	54.2	26.5	16.4	35.7	15.4	40.4	0.31	2.32
Mg-$Li_{0.25}$ (8.7 wt%Li)	53.3	26.3	–	–	15.3	53.3	26.3	15.3	35.3	14.6	38.5	0.32	2.41
Mg-$Li_{0.33}$ (12.5 wt%Li)	51.6	24.9	–	–	14.1	51.6	24.9	14.1	33.8	13.8	36.4	0.32	2.45
$Fe_{0.64}Mn_{0.36}$	207	115	–	–	112	207	115	112	145	85.6	214	0.26	1.70
$Fe_{0.61}Mn_{0.36}Ca_{0.03}$	149	120	–	–	100	149	120	100	130	65.8	169	0.28	1.97
$Fe_{0.61}Mn_{0.36}Mg_{0.03}$	200	117	–	–	104	200	117	104	145	79.1	201	0.27	1.83

Simulation Package (VASP) was used within the projector-augmented wave (PAW) method [12,13] and the generalized gradient approximation (GGA) for the exchange-correlation energy functional in a form suggested by Perdew and Wang [14]. VASP is the most powerful *ab-initio* DFT package available at present based on the pseudopotential concept. It was successfully utilized in many different areas of computational physics and chemistry, to study the structure and phase stability of several materials, mechanical and dynamical properties of various materials systems, liquids, glasses and quasicrystals, magnetism and magnetic nanostructures, semiconductors and insulators, surfaces, interfaces, chemical reactions, catalysis *etc*. [15]. This program calculates the electronic structure and inter-atomic forces determined from first-principles via the Hellmann-Feynman theorem. The stress-strain approach relies on the specific feature of VASP to directly calculate the stress tensor. Once the stress tensor components can be computed by an *ab-initio* method, the elastic constants matrix can be directly derived from the generalized Hooke's law mentioned above. Standard PAW potentials were employed for the elemental constituents of all the alloys considered in the present study. For all the materials considered in this study, the plane wave cutoff energy of 520 eV has been chosen to maintain a high accuracy of the total energy calculations. The lattice parameters and internal positions of the atoms were fully optimized during the double relaxation procedure employed, and consequently, the minima of the total energies with respect to the lattice parameters and internal ionic positions have all been determined. A deformation matrix with different distortion values δ of ± 1% and ± 2% has been applied to both, the hexagonal and cubic crystal structures.

For most of the alloys the $Mg_{35}M_1$ formula unit has been chosen utilizing [3 × 3 × 2] 36-atom *hcp* cell. Such a formula unit corresponds to 2.78 at% of the metal selected as an alloying element in the Mg-alloy. For binary and ternary co-alloys only one atom of each element has been introduced into the Mg-*hcp* lattice placing them randomly apart from each other as far as possible, thus avoiding any spatial segregation of the alloying elements. Due to the wide concentration range of Mg-Li alloys considered in the present study $Mg_{35}Li_1$, $Mg_{30}Li_6$ and $Mg_{33}Li_3$ formula units have been chosen within the 36-atom *hcp* cell, while $Mg_{27}Li_9$, and $Mg_{24}Li_{12}$ formula units as well as Fe-based alloys $Fe_{23}Mn_{13}$, $Fe_{22}Mn_{13}Ca_1$, and $Fe_{22}Mn_{13}Mg_1$ formula units have also been constructed based on the [3 × 3 × 2] 36-atom body-centered cubic (*bcc*) supercell.

3. Results and discussion

All the calculated elastic stiffness values along with bulk, shear, Young's moduli and Poisson's ratio are collected in Table 1. The first line of Table 1 contains the calculated and experimental stiffness values as well as the corresponding elastic moduli for pure Mg. It can be seen that the calculated data agrees well with the experimentally determined values obtained from A. Wazzan et al. [16] which validate the computational approach employed in the present study.

As seen from Table 1, all Mg-based alloys with various metallic element additions as alloying elements except Y-metal, demonstrate a higher Poison's ratio and *B/G* ratio than the corresponding values for pure Mg although to different extents. For example, the highest ductility among all the materials studied has been determined to be in Mg alloyed with Zn, Ca, and substantial amount of Li (up to 12.5 wt%). Ag and Sr also improve the ductility but to noticeably less extent than the above mentioned elements. The least favorable elements with regards to improving the ductility are Zr, Y, and rare earth elements Ce, Nd, and Sm. These elements can be used as additions to alloys exhibiting high initial ductility but mediocre other mechanical properties, such as yield strength or ultimate tensile strength. Alloying with these elements can lead to significant increase in mechanical strengths. For example, several experimental studies have shown that Mg-alloys with Zn and rare earth elements demonstrate unusually high ultimate tensile strengths due to the formation of long period stacking ordered (LPSO) crystal structure [17–19]. Such alloys may combine high mechanical strength along with high ductility, both being very much desirable characteristics for bio-resorbable orthopedic and cardiovascular applications.

Experimental measurements of the elastic stiffness coefficients for several Mg-Li alloys have been reported by A. Wazzan et al. [16]. Among the different alloy compositions considered in [16] the closest compounds to those chosen in the present study are those containing 3.02 and 7.0 at% of Li. Thus, for comparison of the calculated c_{ij} values for 2.78 at% and 8.3 at% of Li with corresponding experimental values from [16] the latter were linearly interpolated and collected in Table 1. It can be seen that there is reasonable agreement between the calculated and experimental data, especially the derivative elastic moduli. Also, calculated c_{ij} values for Mg alloys with Ca, Zn, and Y agree very well with similar calculations reported earlier by S. Ganeshan et al. in [20].

As for the Fe-based alloys, these materials have been chosen since they demonstrate faster degradation than that of pure Fe and in addition, they exhibit good biocompatibility with the physiological body environment [4]. Thus, it can be seen from Table 1, the calculated elastic moduli for Fe-Mn alloy is much higher than Mg alloys. However, at the same time, the calculated *B/G* values for ductility are significantly lower compared to the corresponding values of Mg-based alloys. This can be attributed to the much higher cohesive energy of pure Fe (4.28 eV/at.) and Mn (2.92 eV/at.) in comparison to Mg metal (1.51 eV/at.) [21], thus resulting in higher stiffness values in response to bulk and shear deformations. Incorporation of small amount of Ca and Mg to Fe-Mn alloy slightly improves the ductility but decreases the corresponding elastic moduli due to lower cohesive energies of both Ca and Mg compared to Fe and Mn. The addition of these elements however, enhances the corrosion and are thus determined to be favorable as promising biodegradable iron based alloys. These alloys were also successfully used for binder-jetting 3-D printing of constructs demonstrating promising corrosive and mechanical characteristics suitable for bio-applications such as customized patient-specific bioresorbable scaffolds and implants as reported in [9,10]. The study conducted herein therefore shows the potential of DFT based studies for determining the use of certain select alloying elements for improving the ductility as well as elastic stiffnesses.

4. Conclusions

In the present study, the Density Functional Theory has been used to investigate the influence of alloying effects on the general elastic properties of different biocompatible elements when introduced into the Mg and Fe crystal lattice. The study has shown that alloying of Mg with Zn, Ca, Li, Ag, Sr, and Zr improves the ductility of the alloys, especially alloying of Mg with Zn, Ca, and high percentage of Li, while an addition of Y makes the alloy less ductile than pure Mg. Some ternary and quaternary Mg-based alloys also demonstrate noticeable improvement in ductility. On the other hand, with regards to Fe-based alloys, the Fe-Mn alloy system alloyed with small amount of Ca and Mg demonstrate similar or lower ductility, while the elastic moduli are much higher than the corresponding values determined for pure Mg and Mg based alloys. Thus, the present study demonstrates the ability to identify several alloying elements for improving the overall ductility of the Mg- and Fe-based alloys making them suitable for cardiovascular, bronchotracheal and orthopedic applications as novel bio-resorbable alloys. The studies could be useful for experimentalists to generate novel bioresorbable alloys for all these applications in the future.

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References

[1] J. Nagels, M. Stokdijk, P. Rozing, Stress shielding and bone resorption in shoulder arthroplasty, J. Shoulder Elbow Surg. 12 (2003) 35–39.
[2] M. Staiger, A. Pietak, J. Huadmai, G. Dias, Magnesium and its alloys as orthopedic biomaterials: a review, Biomaterials 27 (2006) 1728–1734.
[3] F. Witte, V. Kaese, H. Haferkamp, E. Switzer, A. Meyer-Lindenberg, C.J. Wirth, H. Windhagen, In vivo corrosion of four magnesium alloys and the associated bone response, Biomaterials 26 (2005) 3557–3563.
[4] O.I. Velikokhatnyi, P.N. Kumta, First-principles studies on alloying and simplified thermodynamic aqueous chemical stability of calcium-, zinc-, aluminum-, yttrium- and iron-doped magnesium alloys, Acta Biomater. 6 (2010) 1698–1704.
[5] E. Willbold, X. Gu, D. Albert, K. Kalla, K. Bobe, M. Brauneis, C. Janning, J. Nellesen, W. Czayka, W. Tillmann, Y. Zheng, F. Witte, Effect of the addition of low rare earth elements (lanthanum, neodymium, cerium) on the biodegradation and biocompatibility of magnesium, Acta Biomater. 11 (2015) 554–562.
[6] M. Pogorielov, E. Husak, A. Solodivnik, S. Zhdanov, Magnesium-based biodegradable alloys: Degradation, application, and alloying elements, Interventional Med. Appl. Sci. 9 (2017) 27–38.
[7] M. Esmaily, J.E. Svensson, S. Fajardo, N. Birbilis, G.S. Frankel, S. Virtanen, R. Arrabal, S. Thomas, L.G. Johansson, Fundamentals and advances in magnesium alloy corrosion, Prog. Mater. Sci. 89 (2017) 92–193.
[8] H. Hermawan, H. Alamdari, D. Mantovani, D. Dubé, Iron–manganese: new class of metallic degradable biomaterials prepared by powder metallurgy, Powder Metall. 51 (2008) 38–45.
[9] D.-T. Chou, D. Wells, D. Hong, B. Lee, H. Kuhn, P.N. Kumta, Novel processing of iron-manganese alloy-based biomaterials by inkjet 3-D printing, Acta Biomater. 9 (2013) 8593–8603.
[10] D. Hong, D.T. Chou, O. Velikokhatnyi, A. Roy, B. Lee, I. Swink, I. Issaev, H.A. Kunn, P.N. Kumta, Binder-jetting 3D printing and alloy development of new biodegradable Fe-Mn-Ca/Mg alloys, Acta Biomater. 45 (2016) 375–386.
[11] S.F. Pugh XCII, Relations between the elastic moduli and the plastic properties of polycrystalline pure metals, Phil. Mag. 45 (1954) 823–843.
[12] G. Kresse, J. Furthmuller, Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set, Phys. Rev. B 54 (1996) 11169–11186.
[13] G. Kresse, J. Furthmuller, Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set, Comp. Mat. Sci. 6 (1996) 15–50.
[14] J.P. Perdew, Y. Wang, Accurate and simple density functional for the electronic exchange energy: generalized gradient approximation, Phys. Rev. B 33 (1986) 8800–8802.
[15] J. Hafner, *Ab-Initio* simulations of materials using VASP: density-functional theory and beyond, J. Comput. Chem. 29 (2008) 2044–2078.
[16] A.R. Wazzan, L.B. Robinson, Elastic constants of magnesium-lithium alloys, Phys. Rev. 155 (1967) 586–594.
[17] D. Egusa, E. Abe, The structure of long period stacking/order Mg–Zn–RE phases with extended non-stoichiometry ranges, Acta Mater. 60 (2012) 166–178.
[18] L.U. Fumina, M.A. Aibina, J. Jiang, D. Yangb, Q. Zhou, Review on long-period stacking-ordered structures in Mg-Zn-RE alloys, Rare Met. 31 (2012) 303–310.
[19] X. Zhao, L. Shi, J. Xu, Mg–Zn–Y alloys with long-period stacking ordered structure: in vitro assessments of biodegradation behavior, Mater. Sci. Eng. C 33 (2013) 3627–3637.
[20] S. Ganeshan, S.L. Shang, Y. Wang, Z.-K. Liu, Effect of alloying elements on the elastic properties of Mg from first-principles calculations, Acta Mater. 57 (2009) 3876–3884.
[21] C. Kittel, Introduction to Solid State Physics, eighth ed., John Wiley & Sons Inc, Hoboken, NJ, 2005.
[22] J. Towns, T. Cockerill, M. Dahan, I. Foster, K. Gaither, A. Grimshaw, V. Hazlewood, S. Lathrop, D. Lifka, G.D. Peterson, R. Roskies, J.R. Scott, N. Wilkins-Diehr, XSEDE: accelerating scientific discovery, Comput. Sci. Eng. 16 (2014) 62–74, http://dx.doi.org/10.1109/MCSE.2014.80.