Empirical mapping of ZrCu-based alloys with valence electrons *versus* transformation temperatures

Weihong Gao¹, Xianglong Meng^{1*}, Gangbing Song², Wei Cai¹ and Liancheng Zhao¹

ABSTRACT An empirical map of martensitic transformation temperatures *versus* average valence electrons per atom (e_v/a) and valence electron concentration (c_v) was developed in order to design ZrCu-based shape memory alloys (SMAs). The martensitic transformation temperatures of about 40 different alloys (Ni, Co, Hf, Ag, Ti, Al, Cr, etc.), covering nearly all possible replacements of Zr or Cu, are exhibited. The relationship between transformation temperature and c_v or electron density (n) was determined. The results indicate that the transformation temperatures of ZrCu-based alloys gradually decrease until reaching an inflection point at $c_v = 0.218$, above which the transformation temperatures go down. A linear dependence of the transformation temperatures of ZrCu-based alloys on the electron density is revealed by data-fitting. Under the guidance of these contour maps describing transformation temperatures and thermal hysteresis, a series of ZrCu-based alloys that can function under different conditions can be designed.

Keywords: ZrCu alloy, shape memory alloys, valence electrons concentration, martensitic transformation temperatures

INTRODUCTION

Shape memory alloys (SMAs) exhibit unique shape memory effects and superelasticity behavior due to their martensitic transformation [1,2]. ZrCu-based alloys undergo a thermoelastic martensitic transformation from a B2 structure to two different monoclinic martensitic structures: one with a base structure (B19') with $P2_1/m$ symmetry and the other with a superstructure (B33) with $Cmcm$ symmetry [3,4]. They are considered as competitive high temperature shape memory alloys (HTSMAs) due to their low fabrication costs and high martensitic transformation temperatures, which are associated with favorable shape memory effects [5,6]. For example, a $Zr_{42.3}Cu_{29.9}Ni_{11}Co_{10.2}Ti_{6.6}$ alloy can achieve a recoverable strain of 3.5% under 8% applied compressive strain, with a high martensitic starting transformation temperature (M_s) of 450 K [4]. In addition, ZrCu-based bulk metallic glass (BMG) matrix composites show enhanced plasticity and overall work hardening

under compressive loading because the B2-structured nanocrystals undergo a martensitic transformation during deformation [7,8]. Therefore, it is necessary to design the chemical composition of such materials to control the martensitic transformation temperatures, in order to acquire high transformation temperatures in HTSMA devices or to obtain B2 phase-BMG composites for applied use [9,10].

The mechanism that allows alloying elements to change their transformation temperatures is dependent upon the electronic structures and the interatomic bonding forces within such alloys [11]. The valence electrons contributed by s + d electrons of the transition metals, or s + p electrons of the non-transition metals, act as adhesives during metallic bonding [12,13]. The strength of this adhesion, which depends on the number (e_v/a), concentration (c_v), density (n) of valence electrons, is relevant to the transformation temperatures of SMAs [11–16]. For ZrCu-based alloys, the relationship between transformation temperature and electronic structure has yet to be quantified, and therefore a guiding empirical map is necessary to design and optimize the central properties in ZrCu-based alloys. In this paper, we have examined the number (e_v/a), concentration (c_v) and density (n) of valence electrons as correlates with the transformation temperatures of various ZrCu-based alloys. Understanding such correlations would significantly benefit the design of ZrCu-based alloys for different application backgrounds.

MATERIALS AND EXPERIMENTAL PROCEDURE

To adjust the Zr/Cu ratio through substitutions of Zr or Cu with Hf, Co, Ti, Ag, Ni, Al or Cr, ZrCu-based alloys were melted using high-purity metals in a non-consumed vacuum arc furnace under Ar. The ingots were then melted six more times to ensure compositional homogeneity (turning the button 180° for each repetition). The samples were annealed in vacuum quartz tubes at 1073 K for

¹ School of Materials Science and Engineering, Harbin Institute of Technology, Harbin 150001, China

² Department of Mechanical Engineering, University of Houston, Houston TX 77204-4006, USA

* Corresponding author (email: xlmeng@hit.edu.cn)

4 h, followed by quenching with water. The phase transformation temperatures of the alloys were determined by differential scanning calorimetry (DSC), using a Diamond DSC calorimeter with a heating/cooling rate of 20 K min⁻¹. Our experimental data, together with previously reported transformation temperatures [4,17–22] of about 40 different alloys covering nearly all replacement elements of Zr or Cu, are listed in Table 1. Phase purity and crystal structures were determined by X-ray diffraction (XRD) using Cu K α radiation at room temperature.

RESULTS AND DISCUSSION

The number of valence electrons can be calculated based on the contributions of the s + d electrons from the transition metals, or the s + p electrons of the non-transition metals [12]. Since both Zr and Cu are transition metals, the number of valence electrons (e_v) for Zr and Cu are 4(5s²4d²) and 11(4s¹3d¹⁰), respectively. Therefore, the average valence electrons per atom (e_v/a) in the equiatomic ZrCu alloy is 7.5. The valence electron concentration (c_v) is defined as the number of valence electrons in the alloy divided by the total electrons in the alloy as calculated by using the following equations [13]

$$\frac{e_v}{a} = f_{Zr}e_v^{Zr} + f_{Cu}e_v^{Cu} + f_T e_v^T + f_Q e_v^Q, \quad (1)$$

$$c_v = \frac{f_{Zr}e_v^{Zr} + f_{Cu}e_v^{Cu} + f_T e_v^T + f_Q e_v^Q}{f_{Zr}Z_{Zr} + f_{Cu}Z_{Cu} + f_T Z_T + f_Q Z_Q}, \quad (2)$$

where f_{Zr} , f_{Cu} , f_T , and f_Q represent the atomic fractions of elements in the alloy for Zr, Cu, ternary, and quaternary elements, respectively. e_v^{Zr} , e_v^{Cu} , e_v^T , and e_v^Q are the corresponding number of valence electrons of Zr, Cu, and the ternary and quaternary elements, respectively. Z_{Zr} , Z_{Cu} , Z_T and Z_Q represent the atomic numbers of Zr, Cu, and the ternary and quaternary elements, respectively. The variations of M_s vs. e_v/a and c_v are plotted in Figs 1a and b, respectively. The calculated e_v/a values for ZrCu-based alloys range from 6.7 to 7.85, while c_v ranges from 0.2036 to 0.2312. The transformation temperatures in ZrCu-based alloys are found mostly in a number of valence electrons per atom in the range of $7.0 \leq e_v/a \leq 7.5$. The transformation temperature data are scattered and no clear relationship between the transformation temperatures and the e_v/a or c_v was observed, although the highest transformation temperatures are observed within this range. However, the transformation temperatures in ZrCu-based SMAs seem to be a function of both e_v/a and c_v . A contour map of martensitic transformation temperature M_s in a wide e_v/a and c_v range

is summarized in Fig. 1c. According to the contours of the two-variable polynomial fitting curve, higher temperature for ZrCu-based SMAs can be achieved at e_v/a values of 7.1 to 7.4, and in a c_v range of 0.205 to 0.220.

Apart from the effects of e_v/a , the variations of M_s and A_s vs. c_v at $e_v/a = 7.5$ is shown in Fig. 2. Among the alloys at the same e_v/a value (7.5), the transformation temperatures are very sensitive to c_v . For ZrCu-based alloys within the statistical data, both M_s and A_s decrease monotonously from temperatures as high as 450 K (575 K) down to as low as 275 K (450 K) for alloys at $c_v = 0.206$ –0.224. This decreased rate appears to change at $c_v = 0.218$. Further increases of c_v cause both M_s and A_s to sharply decrease. The general trend of martensitic transformation equilibrium temperature T_0 ($T_0 = (M_p + A_p)/2$, where M_p and A_p represent the peaks of the martensitic and reverse transformations, respectively) vs. c_v is similar to A_s and M_s , as shown in Fig. 2c. However, when $e_v/a \neq 7.5$, no obvious trend between the transformation temperatures and c_v is present.

The transformation temperature of ZrCu-based alloys decreases with increasing c_v . An increased c_v leads to strengthened bonds, and in turn an enhancement of the B2 structure stability. The valence electron concentration in this structure is mainly determined by d–d interactions of the Cu and Zr electrons [25]. This stabilization originates from the deformation splitting of the electronic density of states peak above the Fermi level induced by the d–d hybridization between Zr and Cu sites, which forms an additional occupied electron state close to E_F and increases the total energy of the B2 phase [26]. The d–d hybridization between Zr and Cu sites becomes stronger as the valence electron concentration increases, which increases the total energy; likewise as the stability of the B2 structure strengthens, M_s decreases. Moreover, a higher valence electron concentration usually results in higher bulk and shear moduli, which for solid state materials is a measure of resistance to volume change and a measure of resistance to shape change, respectively [11–13]. In summary, higher c_v values lead to lower transformation temperatures.

In considering the crystal structure of ZrCu-based alloys, valence electron density (n) which is a function of the number of valence electron (e_v/a) and the unit volume of the crystal (V_{cell}), is a factor for describing transformation temperature variations. This relationship can be expressed as [27]

$$n = \frac{e_v/a}{V_{cell}} \cdot N, \quad (3)$$

where N represents the average number of atoms contained in a unit cell. In order to study the relationship between va-

Table 1 The number of valence electrons per atom e_v/a , valence electrons concentration c_v , martensite start transformation temperature M_s , austenite start transformation temperature A_s and thermal hysteresis ($\Delta T = A_p - M_p$) for ZrCu-based shape memory alloys

Alloy	M_s (K)	A_s (K)	ΔT (K)	e_v/a	c_v	Ref.
Zr ₅₀ Cu ₅₀	358	529	182	7.5	0.2174	Present study
Zr ₅₀ Cu ₅₀	413	—	—	7.5	0.2174	[17]
Zr ₅₀ Cu ₅₀	323	531	190	7.5	0.2174	[23]
Zr ₅₀ Cu ₅₀	368	503	—	7.5	0.2174	[18]
Zr ₅₅ Cu ₄₅	401	532	—	7.15	0.214	[18]
Zr ₅₂ Cu ₄₈	431	526	—	7.36	0.216	[18]
Zr ₄₈ Cu ₅₂	433	519	—	7.64	0.2229	[18]
Zr ₄₅ Cu ₅₅	411	516	—	7.85	0.2312	[18]
Zr _{48.2} Cu ₅₀ Ti _{1.8}	383	561	178	7.5	0.2195	[24]
Zr _{47.2} Cu ₅₀ Ti _{2.8}	323	516	193	7.5	0.2206	[24]
Zr _{46.5} Cu ₅₀ Ti _{3.5}	308	528	220	7.5	0.2214	[24]
Zr _{44.5} Cu ₅₀ Ti _{5.5}	283	453	170	7.5	0.2238	[24]
Zr _{49.6} Cu _{28.2} Ni _{6.8} Co _{15.4}	485	526	82.5	7.15	0.2098	[4]
Zr ₅₀ Cu ₂₅ Ni _{2.5} Co _{22.5}	398	422	53	7.025	0.2101	Present study
Zr ₅₀ Cu ₂₅ Ni ₅ Co ₂₀	483	507	57	7.05	0.207	Present study
Zr ₅₀ Cu ₂₅ Ni _{7.5} Co _{17.5}	564	568	60	7.075	0.2076	Present study
Zr ₅₀ Cu ₂₅ Ni ₁₀ Co ₁₅	603	681	98	7.1	0.2082	Present study
Zr _{42.3} Cu _{29.9} Ni ₁₁ Co _{10.2} Ti _{6.6}	410	450	70	7.26	0.2208	[4]
Zr ₅₀ Cu ₄₈ Ni ₂	464	561	110	7.48	0.2169	Present study
Zr ₅₀ Cu ₄₆ Ni ₄	510	604	111	7.46	0.2165	Present study
Zr ₅₀ Cu ₄₄ Ni ₆	533	653	137	7.44	0.216	Present study
Zr ₅₀ Cu ₄₂ Ni ₈	562	682	141	7.42	0.2156	Present study
Zr ₅₀ Cu ₄₀ Ni ₁₀	587	722	136	7.40	0.2151	Present study
Zr ₅₀ Cu ₄₅ Ni ₅	433	608	—	7.45	0.2161	[23]
Zr ₅₀ Cu ₄₀ Ni ₁₀	536	700	—	7.4	0.2151	[23]
Zr _{50.59} Cu _{29.56} Ni _{19.85}	497	597	—	7.26	0.2113	[19]
Zr ₅₀ Cu ₄₅ Cr ₅	341	432	—	7.25	0.2117	[20]
Zr ₅₀ Cu _{49.5} Ag _{0.5}	433	526	112	7.5	0.2168	Present study
Zr ₅₀ Cu ₄₉ Ag ₁	436	528	118	7.5	0.2163	Present study
Zr ₅₀ Cu ₄₈ Ag ₂	415	515	120	7.5	0.2151	Present study
Cu ₅₀ Zr ₄₈ Hf ₂	440	540	128	7.5	0.2134	Present study
Cu ₅₀ Zr ₄₆ Hf ₄	443	547	132	7.5	0.2096	Present study
Cu ₅₀ Zr ₄₄ Hf ₆	442	557	140	7.5	0.2059	Present study
Cu ₅₀ Zr ₄₂ Hf ₈	436	577	165	7.5	0.2024	Present study
Zr ₅₀ Cu ₄₈ Co ₂	410	485	—	7.46	0.2165	[21]
Zr ₅₀ Cu ₄₇ Co ₃	396	470	—	7.44	0.216	[21]
Zr ₅₀ Cu ₄₆ Co ₄	375	431	—	7.42	0.2156	[21]
Zr ₅₀ Cu ₄₅ Co ₅	355	419	—	7.40	0.2151	[21]
Zr ₅₀ Cu ₄₈ Al ₂	415	503	—	7.34	0.2147	[22]
Zr ₅₀ Cu ₄₆ Al ₄	362	474	—	7.18	0.212	[22]
Zr ₅₀ Cu ₄₄ Al ₆	311	464	—	7.02	0.2093	[22]
Zr ₅₀ Cu ₄₂ Al ₈	309	455	—	6.86	0.2065	[22]
Zr ₅₀ Cu ₄₀ Al ₁₀	306	455	—	6.7	0.2036	[22]

Figure 1 Variations of martensitic transformation start temperature (M_s) (most datas from our studies while partial from Refs. [4,17,18,20–24]) with the number of valence electrons per atom (e_v/a) (a) and valence electron concentration (c_v) (b) of ZrCu-based shape memory alloys, (c) contour views of the curve fitted M_s versus e_v/a and c_v .

Figure 2 Variation of Martensite start temperatures M_s (a) and Austenite start temperatures A_s (b) versus different alloy elements with $e_v/a=7.5$; (c) the relationship between martensitic transformation equilibrium temperature (T_0) and valence electrons concentration c_v .

lence electron densities and transformation temperatures, Zr-Cu-Ni and Zr-Cu-Hf alloys are designed and partial data are selected from Ref. [21]. All the diffraction peaks of the samples can be well indexed to monoclinic martensite (a base structure B19' and a superstructure B33). The B33 martensite phase is the superstructure of the basic structure B19' martensite and consists of four units of B19' structures [28]. Therefore, the variation tendency of the unit-cell volume is based on the lattice parameter of B19' martensite in Zr-Cu-Ni and Zr-Cu-Hf alloys. A linear relationship between the transformation temperatures (A_s and M_s) and the electron density is shown in Fig. 3. In order to better determine the temperature scale corresponding to electron density changes, trends were estimated for the effect of n on T_0 as shown in Fig. 3c. This analysis allows us to write the empirical formula $T_0 = 2158 - 3826n$, where T_0 is the martensitic transformation equilibrium temperature. Based on this equation, T_0 above 1000 K (corresponding to the potential HTSMAs with high transformation temperature) can be obtained if $n < 0.303$, while T_0 close to room temperature can be achieved when $n \approx 0.486$.

It is particularly notable that the transformation hysteresis of ZrCu-based alloys is very broad (183 K for $Zr_{50}Cu_{50}$

alloy), and the martensitic transformation can be considered as non-thermoelastic [29]. The wide thermal hysteresis of SMAs may result in longer response times, as well as small sensitivity and frequency values which are not anticipated for actuator applications. The contour map for the thermal hysteresis behavior vs. c_v and e_v/a is shown in Fig. 4. The darkest area represents a very small thermal hysteresis (about 50 K). When c_v is held constant, the thermal hysteresis distinctly becomes narrower as e_v/a decreases. The small thermal hysteresis is a characteristic of the thermoelastic transformation in SMAs. Normally, SMAs with thermoelastic transformations can exhibit favorable shape memory effects. For example, a $Zr_{42.3}Cu_{29.9}Ni_{11}Co_{10.2}Ti_{6.6}$ alloy with a smaller thermal hysteresis (70 K) than other ZrCu-based alloys can achieve a shape memory effect of approximately 3.5% [4]. In addition, this smaller thermal hysteresis is accompanied by a small energy dissipation derived from the friction of domain rearrangements and phase boundary migrations. Thus, this map demonstrates that to acquire small thermal hysteresis in ZrCu-based alloys, a relatively small e_v/a value is necessary. According to the contours (Figs 1c and 4) of the two-variable polynomial fitting curves, higher transformation temperatures

Figure 3 The XRD patterns of (a) $Zr_{50}Cu_{50-x}Ni_x$ ($x=0, 2, 4, 6, 8, 10$) and (b) $Cu_{50}Zr_{50-x}Hf_x$ ($x=0, 2, 4, 6$) alloys at room temperature. (c) The relationship between martensitic transformation equilibrium temperature (T_0) and electron density (n). (Most data from our studies while partial from Ref. [20]).

Figure 4 Contour views of the curve fitted thermal hysteresis (Most data from our studies while partial from Refs. [4,24,28]).

and smaller thermal hysteresis in ZrCu-based alloys can be achieved with the e_v/a values between 7.1 to 7.2, and c_v values between 0.207 to 0.220, respectively.

CONCLUSIONS

In summary, an empirical map describing transformation temperature *vs.* e_v/a and c_v is described for designing Zr-Cu-based systems. The transformation temperatures of Zr-Cu-based alloys decrease with increasing c_v when $e_v/a = 7.5$, which can be interpreted that increased valence electron concentration related to the total density of states at the Fermi level leads to the stabilization of B2 structures. A linear relationship between transformation temperature and valence electron density was also determined. This study yields further understanding of the influence that chemical composition has on the transformation temperatures of ZrCu-based alloys, enabling more effective alloy design.

Received 14 January 2016; Accepted 23 February 2016;
published online 29 February 2016

- Otsuka K, Wayman CM. Shape Memory Materials. Cambridge: Cambridge University Press, 1998
- Emre A, Osman EO, Haluk EK. Experimental investigation and modeling of the loading rate and temperature dependent super-elastic response of a high performance shape-memory alloy. *Smart Mater Struct*, 2015, 24: 075020
- Ma J, Karaman I, Noebe RD. High temperature shape memory alloy. *Int Mater Rev*, 2010, 55: 257–315
- Firstov GS, Humbeeck JV, Koval YN. Comparison of high temperature shape memory behavior for ZrCu-based, Ti-Ni-Zr and Ti-Ni-Hf alloys. *Scr Mater*, 2004, 50: 243–248
- Meng XL, Gao WH, Gao ZY, Cai W, Zhao LC. Substructure and interface of the superstructure martensitic in $Zr_{50}Cu_{50}$ high temperature shape memory alloy. *Mater Lett*, 2014, 117: 221–224
- Gao WH, Meng XL, Cai W, Zhao LC. Martensite structure and phase transformation of quaternary ZrCuAlCo high temperature

- shape memory alloys. *J. Alloys Comp*, 2014, 607: 99–103
- Hofmann DC. Shape memory bulk metallic glass composites. *Science*, 2010, 329: 1294
- Pauly S, Liu G, Wang G, *et al.* Modeling deformation behavior of Cu-Zr-Al bulk metallic glass matrix composites. *Appl Phys Lett*, 2009, 95: 101906
- Song GB, Ma N, Lee HJ, Arnold S. Design and control of a proof-of-concept variable area exhaust nozzle using shape-memory alloy actuators. *Smart Mater Struct*, 2007, 16: 1342–1347
- Glock S, Michaud VT. Thermal and damping behaviour of magnetic shape memory alloy composites. *Smart Mater Struct*, 2015, 24: 065025
- Zarinejad M, Liu Y. Dependence of transformation temperatures of NiTi-based shape-memory alloys on the number and concentration of valence electrons. *Adv Funct Mater*, 2008, 18: 1–6
- Zarinejad M, Liu Y, Tong YX. Transformation temperature changes due to second phase precipitation in NiTi-based shape memory alloys. *Intermetallics*, 2009, 17: 914–919
- Zarinejad M, Liu Y. Dependence of Transformation Temperatures of Shape-memory Alloys on the Number and Concentration of Valence Electrons. New York: Nova Science Publishers Inc, 2010: 339–360
- Huang YJ, Hu QD, Li JG. Design in Ni-Mn-In magnetic shape-memory alloy using compositional maps. *Appl Phys Lett*, 2012, 101: 222403
- Sutou Y, Imano Y, Koeda N, *et al.* Magnetic and martensitic transformations of NiMnX (X=In,Sn,Sb)...ferromagnetic shape memory alloys. *Appl Phys Lett*, 2004, 85: 4358
- Jin X, Marioni M, Bono D, Allen SM, O'Handley RC. Empirical mapping of Ni-Mn-Ga properties with composition and valence electron concentration. *J Appl Phys*, 2002, 91: 8222–8224
- Koval YN, Firstov GS, Kotko AV. Martensitic transformation and shape memory effect in Zr-Cu intermetallic compound. *Scr Metall et Mater*, 1992, 27: 1611–1616
- Biffi CA, Figini A, Tuissi A. Influence of compositional ratio on microstructure and martensitic transformation of CuZr shape memory alloys. *Intermetallics*, 2014, 46: 4–11
- Firstov GS, Koval YN, Humbeeck JV, *et al.* Phase transformations in Zr–29.56 at.% Cu–19.85 at.%Ni melt-spun high-temperature shape memory alloy. *Mater Sci Eng A*, 2006, 438–440: 816–820
- Biffi CA, Figini A, Tuissi A. CuZr based shape memory alloys: effect of Cr and Co on the martensitic transformation. *Mater Sci Forum*, 2013, 738–739: 167–171
- Javida FA, Mattern N, Pauly S, Eckert J. Martensitic transformation and thermal cycling effect in Cu-Co-Zr alloys. *J Alloys Comp*, 2011, 509S: S334–S337
- Meng FQ, Tsuchiya K, Ii Seiichiro, Yokoyama Y. Influence of Ni on stability of martensitic transformation in $Zr_{50}Cu_{50-x}Ni_x$. *J Alloys Comp*, 2013, 577S: S136–S140
- Meng FQ, Tsuchiya K, Yin FX, Ii S, Yokoyama Y. Influence of Al on stability of martensitic transformation in $Zr_{50}Cu_{50-x}Al_x$. *J Alloys Comp*, 2012, 522: 136–140
- Koval YN, Firstov GS, Kotko AV, Delaey L, Humbeeck JV. The influence of Ni and Ti on the martensitic transformation temperature and shape memory effect of the intermetallic compound ZrCu. *Scr Metall et Mater*, 1994, 31: 799
- Firstov GS, Timoshevskii AN, Koval YN, Kalkuta S, Humbeeck JV. Phase stability during martensitic transformation in ZrCu intermetallics: crystal and electronic structure aspects. *ESOMAT*, 2009, 02008
- Zhalko-Titarenkmo AV, Yevlashinva ML, Antonovb VN, *et al.* Electronic and crystal structure of the ZrCu intermetallic compound close to the point of structural transformation. *Phys Status Solidi*

- B, 1994, 184: 122
- 27 Wang RL, Yan JB, Xiao HB, *et al.* Effect of electron density on the martensitic transition in Ni-Mn-Sn alloys. *J Alloys Comp*, 2011, 509: 6834–6837
- 28 Seo JW, Schryvers D. TEM investigation of the microstructure and defects of CuZr martensite. Part I: morphology and twin systems. *Acta Mater*, 1998, 46: 1165–1175
- 29 Firstov GS, Humbeeck JV, Koval YN. Peculiarities of the martensitic transformation in ZrCu intermetallic compound-potential high temperature SMA. *J Phys IV*, 2001, 11: 481–486

Acknowledgments This work was supported by the National Natural

Science Foundation of China (51171052 and 51322102), the Key Projects of Chinese National Programs for Fundamental Research and Development (2011CB012904 and 2012CB619400), the Doctoral Program Foundation of Institutions of Higher Education of China (20112302130006) and the Fundamental Research Funds for the Central Universities (HIT. BRET III 201201).

Author contributions Gao W, Meng X, Song G, Cai W and Zhao L designed the research. Gao W performed the experiments. Gao W and Meng X wrote the paper.

Conflict of interest The authors declare that they have no conflict of interest.

Weihong Gao is currently a PhD candidate in the Department of Material Physics and Chemistry at Harbin Institute of Technology, China. She received his BSc degree and MSc degree majored in material physics and chemistry at Harbin Engineering University. Her current research is mainly on martensite phase transformation; microstructure and interface of high temperature shape memory alloys.

Xianglong Meng is currently a professor at Harbin Institute of Technology. He obtained his PhD degree from Harbin Institute of Technology in 2004. His research interests focus mainly on high temperature shape memory alloys, martensitic transformation and microstructure.

ZrCu基合金马氏体相变温度与价电子经验图谱

高卫红, 孟祥龙, 宋钢兵, 蔡伟, 赵连城

摘要 本文建立了一个关于马氏体相变温度和价电子数及电子浓度的经验图谱并设计了一系列ZrCu基形状记忆合金. 这些相变温度包括了所有报道过的经Ni、Co、Hf、Ag、Ti、Al、Cr等掺杂替换Zr或者Cu原子的约40种合金. 反映了转变温度和电子浓度或者电子密度之间的关系. 结果显示ZrCu基合金的转变温度逐渐下降, 当 $c_v > 0.218$ 时, 相变温度急剧下降. ZrCu基合金的马氏体相变温度与电子密度呈线性关系. 基于相变温度和滞后图谱的结果可以设计出在不同条件下工作的ZrCu基合金.