Machine learning-based prediction of elastic properties of amorphous metal alloys

1. Artificial neural network learning method

The artificial neural network (ANN) is learned by adjusting the values of all weights taking into account the error between the output neuron and the required result [S. Haykin, Neural networks and learning machines, third ed., Pearson Education Inc., New Jersey, 2009]. The output error ξ_{err} of the ANN is defined by the expression:

$$\xi_{err} = \frac{1}{2}\left(n_1^{(4)}(l) - L_l\right)^2. \tag{1}$$

Here $n_1^{(4)}$ is the value of the output neuron for lth element from the training set; L_l is the required value of the output neuron for the lth element from the training set. The adjustment of weights is carried out as follows:

$$w_{ij}^{(k),new} = w_{ij}^{(k)} - \gamma \frac{\partial \xi_{err}}{\partial w_{ij}^{(k)}}, \tag{2}$$

where γ is the learning rate, the value of which is usually chosen in the interval $[0; 1]$. In the present work, the ANN learning rate is $\gamma = 0.3$. The partial derivative of the error ξ_{err} with respect to the weight $w_{ij}^{(k)}$ is calculated by the chain rule

$$\frac{\partial \xi_{err}}{\partial w_{ij}^{(k)}} = \frac{\partial \xi_{err}}{\partial n_i^{(k)}} \cdot \frac{\partial n_i^{(k)}}{\partial W_i^{(k)}} \cdot \frac{\partial W_i^{(k)}}{\partial w_{ij}^{(k)}}. \tag{3}$$

In the case of the output layer neuron $n_1^{(4)}$, from (1) it follows that the derivative of the error $\partial \xi_{err}/\partial n_1^{(4)}$ is

$$\frac{\partial \xi_{err}}{\partial n_1^{(4)}} = n_1^{(4)}(l) - L_l. \tag{4}$$

In the case of neurons in the hidden layers, the calculation of the error gradient is carried out recursively with the known value of the error on the output layer:

$$\frac{\partial \xi_{err}}{\partial n_i^{(k)}} = \frac{\partial \xi_{err}}{\partial W_i^{(k)}} \cdot \frac{\partial W_i^{(k)}}{\partial n_i^{(k)}}. \tag{5}$$

In Eq. (3), the derivative of the output value of the neuron with respect to its input value $\partial n_i^{(k)}/\partial W_i^{(k)}$ is equal to the derivative of the activation function:

$$\frac{\partial n_i^{(k)}}{\partial W_i^{(k)}} = f(W_i^{(k)})[1 - f(W_i^{(k)})]. \tag{6}$$

The derivative $\partial W_i^{(k)}/\partial w_{ij}^{(k)}$ in (3) is equal to the neuron output $n_i^{(k)}$:

$$\frac{\partial W_i^{(k)}}{\partial w_{ij}^{(k)}} = n_i^{(k)}. \tag{7}$$

Thus, from (2)–(7) it follows that the weights are updated according to the expression

$$w_{ij}^{(k),new} = w_{ij}^{(k)} - \gamma \delta_i n_i^{(k)} \frac{e^{-W_i^{(k)}}}{\left[1 + e^{-W_i^{(k)}}\right]^2}, \tag{8}$$

where

$$\delta_i = \begin{cases} n_1^{(4)}(l) - L_l & \text{if } i \text{ is the output layer neuron} \\ \sum_j w_{ij}^{(k)} \delta_j & \text{if } i \text{ is a neuron of the hidden layers.} \end{cases}$$

Thus, gradient descent reduces the error in the weights.

2. List of materials and its physical characteristics

Table 1: Mechanical characteristics as well as physical and chemical parameters of amorphous metal alloys: the molar mass M, the number of components n in the alloy, the yield stress σ_y, the glass transition temperature T_g, the Young's modulus E. These data are taken from Ref. [R.T. Qu et al., Journal of Alloys and Compounds 637 (2015) 44]. The values predicted by the ANN are shown in bold.

No	Compositions	M, g/mol	n	σ_y, GPa	T_g, K	E, GPa
	Al-based					
1	$Al_{35}La_{33}Gd_{17}Ni_{10}Co_5$	9083.08	5	1.05	560	**62**
2	$Al_{35}La_{30}Ce_{20}Ni_{15}$	8794.24	4	1.16	542	**66**
3	$Al_{35}La_{33}Er_{17}Co_{15}$	9861	4	0.82	586	**54**
4	$Al_{40}La_{35}Y_{10}Ni_{15}$	7710.41	4	1.31	586	**71**
5	$(Al_{0.84}Y_{0.09}Ni_{0.05}Co_{0.02})_{95}Sc_5$	3528.81	5	1.51	560	**79**
6	$Al_{88}Ni_9Ce_2Fe_1$	3238.69	4	1.35	520	**72**
	Au-based					
7	$Au_{49}Ag_{5.5}Pd_{2.3}Cu_{26.9}Si_{16.3}$	12656.58	5	1.02	403	**62**
8	$Au_{45}Cu_{30.5}Ag_{7.5}Si_{17}$	12088.11	4	0.95	399	73.2
9	$Au_{50}Cu_{25.5}Ag_{7.5}Si_{17}$	12755.21	4	0.94	377	65
10	$Au_{55}Cu_{20.5}Ag_{7.5}Si_{17}$	13422.32	4	0.9	371	63.9
11	$Au_{55}Cu_{25}Si_{20}$	12983.52	3	1	348	70
12	$Au_{60}Cu_{15.5}Ag_{7.5}Si_{17}$	14089.42	4	0.83	359	55
13	$Au_{65}Cu_{10.5}Ag_{7.5}Si_{17}$	14756.52	4	0.73	342	48
14	$Au_{70}Cu_{5.5}Ag_{7.5}Si_{17}$	15423.62	4	0.64	339	47
	Ca-based					
15	$Ca_{47}Mg_{19}Zn_7Cu_{27}$	4518.93	4	0.34	393	**41**
16	$Ca_{57}Mg_{19}Cu_{24}$	4271.35	3	0.55	387	38
17	$Ca_{65}Li_{9.96}Mg_{8.54}Zn_{16.5}$	6450.98	4	0.53	320	23
18	$Ca_{65}Mg_{15}Zn_{20}$	4277.45	3	0.3	378	**39**
19	$Ca_{65}Mg_{8.54}Li_{9.96}Zn_{16.5}$	6450.98	4	0.33	317	**41**
	Co-based					
20	$Co_{43}Fe_{20}Ta_{5.5}B_{31.5}$	4986.79	4	5.19	910	268
21	$Co_{43}Fe_5Cr_{15}Mo_{14}C_{15}B_6Er_2$	5516	7	5.2	844	**243**
22	$[(Co_{0.6}Fe_{0.4})_{0.75}B_{0.2}Si_{0.05}]_{96}Nb_4$	4868.26	5	4.17	823	210
23	$[(Co_{0.7}Fe_{0.3})_{0.75}B_{0.2}Si_{0.05}]_{96}Nb_4$	4890.49	5	4.13	820	200
24	$[(Co_{0.8}Fe_{0.2})_{0.75}B_{0.2}Si_{0.05}]_{96}Nb_4$	4912.73	5	4.1	813	200
25	$[(Co_{0.9}Fe_{0.1})_{0.75}B_{0.2}Si_{0.05}]_{96}Nb_4$	4934, 96	5	3, 98	803	190
26	$Co_{41}Cr_{15}Mo_{14}C_{15}B_{15}$	4881.69	5	4.79	871	234
27	$Co_{46}Cr_{15}Mo_{14}C_{10}B_{15}$	5116.3	5	4.65	856	234
28	$Co_{46}Cr_{15}Mo_{14}C_{15}B_{10}$	5122.3	5	4.79	843	221
29	$Co_{48}Cr_{15}Mo_{14}C_{16}B_7$	5219.74	5	4.53	825	217
30	$Co_{50}Cr_{15}Mo_{14}C_{10}B_{11}$	5308.79	5	4.29	827	220
31	$Co_{50}Cr_{15}Mo_{14}C_{15}B_6$	5314.79	5	4.42	810	210
32	$Co_{50}Cr_{15}Mo_{14}C_{18}B_3$	5318.39	5	4.5	801	209
33	$Co_{47}Ir_{10}Ta_8B_{35}$	6518	4	5.88	929	**261**
34	$Co_{54.5}Ta_8B_{37.5}$	5064.86	3	5, 75	970	249
35	$Co_{55}Ta_{10}B_{35}$	5429, 19	3	6, 02	975	**262**
36	$Co_{56}Ta_9B_{35}$	5307, 18	3	5, 97	961	247
37	$Co_{57}Ta_8B_{35}$	5185, 16	3	5, 88	951	240
38	$Co_{58}Ta_7B_{35}$	5063, 15	3	5.8	945	241
39	$Co_{59}Ta_6B_{35}$	4941, 13	3	5.72	934	**253**
40	$Co_{59.5}Ta_8B_{32.5}$	5305, 47	3	5.23	928	234
41	$Co_{60}Ta_5B_{35}$	4819, 12	3	5, 63	930	**250**
42	$Co_{60}Nb_8B_{32}$	4625, 2	3	5, 34	923	**240**
43	$Co_{61}Nb_8B_{31}$	4673, 32	3	5, 29	913	**239**
44	$Co_{62}Nb_8B_{30}$	4721, 44	3	5, 23	895	**236**
45	$Co_{63}Nb_8B_{29}$	4769, 56	3	5, 01	888	**229**

Table 2: Continue of Table 1.

No	Compositions	M, g/mol	n	σ_y, GPa	T_g, K	E, GPa
46	$Co_{64}Nb_8B_{28}$	4817, 68	3	4, 7	885	**218**
	Cu-based					
47	$Cu_{42.5}Zr_{40}Ga_{7.5}$	6872, 59	3	2, 13	744	111
48	$Cu_{43}Zr_{43}Al_7Ag_7$	6907, 07	4	2, 02	680	**92**
49	$Cu_{43}Zr_{43}Al_7Be_7$	7340, 48	4	1, 82	723	**104**
50	$Cu_{45}Zr_{46}Al_7Ti_2$	7427, 19	3	1, 72	733	**94**
51	$Cu_{45}Zr_{48}Al_7$	7427, 19	3	1, 72	733	**89**
52	$Cu_{46}Zr_{42}Al_7Y_5$	7387, 92	4	1, 6	672	85
53	$Cu_{46}Zr_{54}$	7849, 21	2	1, 4	696	84
54	$(Cu_{0.5}Zr_{0.5})_{95}Al_5$	7486, 48	3	1, 82	693	90
55	$Cu_{48}Zr_{52}$	7793, 86	2	1, 57	676	**81**
56	$Cu_{50}Zr_{41}Ti_9$	7348, 29	3	1, 89	671	**97**
57	$Cu_{50}Zr_{43}Al_7$	7288, 8	3	2, 17	731	**111**
58	$Cu_{50}Zr_{44}Ti_6$	7478, 36	3	1, 84	681	**95**
59	$Cu_{50}Hf_{43}Al_7$	11041, 24	3	2, 2	774	113
60	$Cu_{50}Zr_{45}Al_5$	7417, 29	3	1, 89	701	102
61	$Cu_{50}Zr_{50}$	7738, 5	2	1, 92	733	85
62	$Cu_{52}Zr_{48}$	7683, 14	2	1, 71	684	**88**
63	$Cu_{52.5}Zr_{42.5}Ga_5$	7561, 8	3	1, 94	733	105
64	$Cu_{54}Zr_{27}Ti_9Be_{10}$	6415, 46	4	2, 5	721	**129**
65	$Cu_{54}Zr_{22}Ti_{18}Ni_6$	6652, 18	4	2, 13	712	**110**
66	$Cu_{54}Zr_{46}$	7627, 79	2	1, 75	694	**89**
67	$Cu_{55.5}Zr_{27.75}Ti_{9.25}Be_{7.5}$	6568, 63	4	2, 4	720	**124**
68	$Cu_{55}Zr_{30}Ti_{10}Co_5$	7005, 09	4	2, 31	714	130
69	$Cu_{55}Zr_{39}Ti_6$	7339, 97	3	1, 63	678	**84**
70	$Cu_{55}Zr_{40}Ga_5$	7492, 61	3	2, 03	736	109
71	$Cu_{57.5}Hf_{27.5}Ti_{15}$	9280, 38	3	1, 94	729	103
72	$Cu_{57.5}Zr_{40}Ga_{2.5}$	7477, 16	3	1, 91	723	105
73	$Cu_{59}Zr_{34}Ti_7$	7185, 9	3	1, 51	710	**79**
74	$Cu_{60}Hf_{10}Zr_{20}Ti_{10}$	7900, 81	4	1, 95	754	101
75	$Cu_{60}Hf_{25}Ti_{15}$	8993, 02	3	2, 16	730	**111**
76	$Cu_{60}Hf_{30}Ti_{10}$	9646, 13	3	2, 16	725	124
77	$Cu_{60}Zr_{10}Hf_{15}Ti_{15}$	8120, 36	4	2, 14	726	**110**
78	$Cu_{60}Zr_{20}Hf_{10}Ti_{10}$	7900, 81	4	2, 05	754	101, 1
79	$Cu_{60}Zr_{22}Ti_{18}$	6681, 29	3	2, 06	721	**105**
80	$Cu_{60}Zr_{33}Ti_7$	7158, 22	3	2, 16	722	95, 7
81	$Cu_{60}Zr_{37}Ti_3$	7331, 65	3	2, 09	728	**107**
82	$Cu_{60}Zr_{30}Ti_{10}$	7028, 15	3	2, 15	713	**110**
83	$Cu_{61}Zr_{34}Ti_5$	7217, 26	3	1, 79	719	**92**
84	$Cu_{62}Zr_{38}$	7406, 36	2	1, 83	732	**93**
85	$Cu_{64}Zr_{36}$	7351, 01	2	2	787	92
86	$Cu_{66}Hf_{34}$	10262, 7	2	2, 1	784	**108**
	Fe-based					
87	$[(Fe_{0.5}Co_{0.5})_{0.75}B_{0.2}Si_{0.05}]_{96}Nb_4$	4846, 02	5	4, 21	820	210
88	$[(Fe_{0.6}Co_{0.1}Ni_{0.3})_{0.75}B_{0.2}Si_{0.05}]_{96}Nb_4$	4818, 61	6	4, 07	792	205
89	$[(Fe_{0.6}Co_{0.2}Ni_{0.2})_{0.75}B_{0.2}Si_{0.05}]_{96}Nb_4$	4820, 33	6	4, 16	800	210
90	$[(Fe_{0.6}Co_{0.3}Ni_{0.1})_{0.75}B_{0.2}Si_{0.05}]_{96}Nb_4$	4822, 06	6	4, 2	813	210
91	$[(Fe_{0.6}Co_{0.4})_{0.75}B_{0.2}Si_{0.05}]_{96}Nb_4$	4823, 79	5	4, 25	825	210
92	$[(Fe_{0.6}Ni_{0.4})_{0.75}B_{0.2}Si_{0.05}]_{96}Nb_4$	4816, 88	5	4, 01	770	203
93	$[(Fe_{0.7}Co_{0.3})_{0.75}B_{0.2}Si_{0.05}]_{96}Nb_4$	4801, 55	5	4, 2	828	210
94	$[(Fe_{0.8}Co_{0.1}Ni_{0.1})_{0.75}B_{0.2}Si_{0.05}]_{96}Nb_4$	4777, 59	6	4, 18	818	208
95	$[(Fe_{0.8}Co_{0.2})_{0.75}B_{0.2}Si_{0.05}]_{96}Nb_4$	4779, 32	5	4, 17	830	205
96	$(Fe_{0.76}Si_{0.096}B_{0.084}P_{0.06})_{99.9}Cu_{0.1}$	4792, 06	5	3, 23	785	158
97	$(Fe_{0.9}Co_{0.1})_{64.25}Mo_{14}C_{15}B_6Er_{0.75}$	5321, 51	6	4	781	193
98	$(Fe_{0.9}Co_{0.1})_{64.5}Mo_{14}C_{15}B_6Er_{0.5}$	5293, 74	6	4, 1	790	192
99	$(Fe_{0.9}Co_{0.1})_{64.75}Mo_{14}C_{15}B_6Er_{0.25}$	5265, 96	6	3, 9	782	193
100	$(Fe_{0.9}Co_{0.1})_{64.875}Mo_{14}C_{15}B_6Er_{0.125}$	5252, 07	6	3, 95	781	193
101	$(Fe_{0.9}Co_{0.1})_{64}Mo_{14}C_{15}B_6Er_1$	5349, 29	6	4	776	196
102	$Fe_{65}Mo_{14}C_{15}B_6$	5218, 11	4	3, 8	789	195
103	$Fe_{41}Co_7Cr_{15}Mo_{14}C_{15}B_6Y_2$	5248, 12	7	3, 5	838	**179**
104	$Fe_{48}Cr_{15}Mo_{14}C_{15}B_6Er_2$	5383, 21	6	4, 2	843	213
105	$Fe_{48}Cr_{15}Mo_{14}C_{15}B_6Y_2$	5226, 5	6	3, 2	839	**165**
106	$Fe_{50}Cr_{15}Mo_{14}C_{15}B_6$	5160, 38	5	4, 17	829	217
107	$Fe_{50}Ni_{30}P_{13}C_7$	5039, 79	4	2, 13	640	**109**
108	$Fe_{53}Cr_{15}Mo_{14}Er_1C_{15}B_6$	5495, 17	6	4, 2	860	195
109	$Fe_{55}Ni_{25}P_{13}C_7$	5025, 54	4	2, 36	649	**121**
110	$Fe_{59}Cr_6Mo_{14}C_{15}B_6$	5195, 02	5	4, 4	806	204
111	$Fe_{60.5}Cr_4Mo_{14}C_{15}B_6Er_{0.5}$	5258, 42	6	4	803	202
112	$Fe_{60}Ni_{20}P_{13}C_7$	5011, 3	4	2, 51	653	**128**
113	$Fe_{61}Mn_{10}Cr_4Mo_6Er_1C_{15}B_6$	5151, 83	7	4, 16	870	193
114	$Fe_{62}Cr_3Mo_{10}P_{12}C_{10}B_3$	5102	6	3, 4	744	172
115	$Fe_{63}Cr_3Mo_{10}P_{12}C_{10}B_2$	5147, 04	6	3, 4	735	178
116	$Fe_{63}Cr_3Mo_{10}P_{12}C_7B_5$	5143, 44	6	3, 4	751	173
117	$Fe_{63}Cr_3Mo_{10}P_{12}C_8B_4$	5144, 64	6	3, 4	745	175
118	$Fe_{63}Cr_3Mo_{10}P_{12}C_9B_3$	5145, 84	6	3, 5	739	175
119	$Fe_{63}Mo_{14}C_{15}B_6Er_2$	5440, 94	5	4	777	204
120	$Fe_{64}Cr_3Mo_{10}P_{10}C_{10}B_3$	5151, 75	6	3, 4	729	176

Table 3: Continue of Table 1.

No	Compositions	M, g/mol	n	σ_y, GPa	T_g, K	E, GPa
121	$Fe_{65}Ni_{15}P_{13}C_7$	4997, 06	4	2, 67	657	**136**
122	$Fe_{66}Cr_3Mo_{10}P_8C_{10}B_3$	5201, 49	6	3, 4	721	177
123	$Fe_{68}Cr_3Mo_{10}P_6C_{10}B_3$	5251, 23	6	3, 5	714	180
124	$Fe_{70}Ni_{10}P_{13}C_7$	4982, 82	4	2, 91	661	**148**
125	$Fe_{75}Ni_5P_{13}C_7$	4968, 58	4	3, 01	667	**153**
126	$Fe_{76}Si_{9.6}B_{8.4}P_6$	4790, 5	4	3, 21	783	165
127	$Fe_{80}P_{13}C_7$	4954, 33	3	3, 14	669	137, 3
	Rare earth-based					
128	$Ce_{70}Al_{10}Ni_{10}Cu_{10}$	11300, 33	4	0, 49	359	30
129	$Ce_{70}Cu_{20}Al_{10}$	11348, 86	3	0, 49	341	31
130	$Dy_{55}Al_{25}Co_{20}$	10790, 7	3	0, 72	635	61
131	$Er_{55}Al_{25}Co_{20}$	11052, 45	3	1, 12	663	71
132	$Gd_{55}Al_{25}Co_{20}$	10501, 95	3	0, 73	585	**51**
133	$Ho_{55}Al_{25}Co_{20}$	10924, 37	3	0, 87	649	67
134	$La_{45}Al_{40}Ni_{15}$	8210, 41	3	1, 25	540	**69**
135	$La_{50}Al_{35}Ni_{15}$	8770, 03	3	1, 11	532	**63**
136	$La_{55}Al_{25}Ni_{20}$	9488, 21	3	0, 52	476	**45**
137	$La_{55}Al_{25}Co_{20}$	9493	3	0, 99	477	41
138	$La_{55}Al_{25}Cu_{10}Ni_5Co_5$	9537, 93	5	0, 5	466	42
139	$La_{57.5}Al_{32.5}C_{10}$	8984, 07	3	1, 06	577	44, 8
140	$La_{60}Al_{30}C_{10}$	9263, 88	3	0, 96	562	43, 1
141	$La_{62}Al_{14}Cu_{24}$	10514, 99	3	0, 48	401	**44**
142	$La_{62}Al_{14}Cu_{20}Ag_4$	10692, 27	4	0, 61	404	**48**
143	$La_{62}Al_{14}Ag_{11.7}Ni_5Co_5Cu_{2.3}$	10986, 23	6	0, 65	422	35
144	$La_{62.5}Al_{27.5}C_{10}$	9543, 69	3	0, 95	556	42, 5
145	$La_{65}Al_{25}C_{10}$	9823, 5	3	0, 89	526	39, 2
146	$La_{66}Al_{14}Cu_{10}Ni_{10}$	10767, 9	4	0, 56	414	**47**
147	$La_{67.5}Al_{22.5}C_{10}$	10103, 31	3	0, 76	507	37, 7
148	$La_{68.5}Ni_{16}Al_{14}Co_{1.5}$	10920, 26	4	0, 35	445	**42**
149	$Lu_{39}Al_{25}Co_{20}Y_{16}$	10099, 41	4	1, 89	687	**99**
150	$Lu_{45}Y_{10}Al_{25}Co_{20}$	10615, 78	4	1, 89	689	**98**
151	$Nd_{55}Al_{25}Co_{20}$	9786, 4	3	1	525	**60**
152	$Nd_{60}Al_{10}Fe_{20}Co_{10}$	10630, 45	4	0, 45	493	51
153	$Pr_{55}Al_{25}Co_{20}$	9603, 13	3	1, 01	509	46
154	$Tb_{55}Al_{25}Co_{20}$	10594, 09	3	0, 83	612	60
155	$Tm_{39}Al_{25}Co_{20}Y_{16}$	9864, 13	4	1, 96	664	77, 5
156	$Y_{55}Al_{25}Co_{20}$	6743, 03	3	1, 2	633	**66**
157	$Yb_{62.5}Zn_{15}Mg_{17.5}Cu_5$	12538, 99	4	0, 45	381	27
	Hf-based					
158	$Hf_{46}Nb_2Cu_{29.25}Ni_{9.75}Al_{13}$	11178, 09	5	2, 53	795	117
159	$Hf_{48}Cu_{29.25}Ni_{9.75}Al_{13}$	11349, 26	4	2, 5	780	116
160	$Hf_{49}Ta_2Cu_{27.75}Ni_{9.25}Al_{12}$	11738	5	2, 49	793	115
161	$Hf_{50}Ni_{25}Al_{25}$	11066, 37	3	2, 73	857	**143**
162	$Hf_{51}Cu_{27.75}Ni_{9.25}Al_{12}$	11733, 08	4	2, 42	773	113
163	$Hf_{55}Ni_{25}Al_{20}$	11823, 92	3	2, 57	828	**135**
164	$Hf_{62}Ni_{25}Al_{13}$	12884, 47	3	2, 29	779	112
	Mg-based					
165	$Mg_{60}Ni_{25}Gd_{15}$	5284, 39	3	0, 87	453	**54**
166	$(Mg_{61}Cu_{28}Gd_{11})_{97}Cd_3$	5179, 13	4	0, 845	426	53
167	$(Mg_{61}Cu_{28}Gd_{11})_{98}Cd_2$	5116, 63	4	0, 85	426	53
168	$(Mg_{61}Cu_{28}Gd_{11})_{99.5}Cd_{0.5}$	5022, 89	4	0, 816	424	51
169	$(Mg_{61}Cu_{28}Gd_{11})_{99}Cd_1$	5054, 14	4	0, 84	425	52
170	$Mg_{61}Cu_{28}Gd_{11}$	4991, 64	3	1, 08	422	52, 2
171	$Mg_{65}Ni_{25}Gd_{10}$	4619, 66	3	0, 88	441	**55**
172	$Mg_{65}Ni_{20}Gd_{15}$	5112, 44	3	0, 91	456	**56**
173	$Mg_{65}Cu_{10}Ag_5Gd_{10}Ni_{10}$	4914, 06	5	1, 01	428	72
174	$Mg_{65}Cu_{12.5}Ag_5Gd_{10}Ni_{7.5}$	4926, 19	5	0, 97	428	70
175	$Mg_{65}Cu_{15}Ag_5Gd_{10}Ni_5$	4938, 32	5	0, 9	422	68
176	$Mg_{65}Cu_{17.5}Ag_5Gd_{10}Ni_{2.5}$	4950, 46	5	0, 84	421	67
177	$Mg_{65}Cu_{20}Ag_5Gd_{10}$	4962, 59	4	0, 82	419	65
178	$Mg_{70}Ni_{20}Gd_{10}$	4447, 72	3	0, 97	453	**57**
179	$Mg_{70}Ni_{15}Gd_{15}$	4940, 5	3	0, 96	464	**57**
180	$Mg_{75}Ni_{15}Gd_{10}$	4275, 78	3	0, 93	463	**56**
181	$Mg_{75}Ni_{10}Gd_{15}$	4768, 56	3	0, 88	465	**55**
182	$Mg_{65}Cu_{20}Y_{15}$	4184, 33	3	0, 82	420	69
183	$Mg_{65}Cu_{25}Gd_{10}$	4740, 98	3	0, 83	425	51
184	$Mg_{65}Cu_{25}Tb_{10}$	4757, 73	3	0, 8	417	51
185	$Mg_{65}Cu_{25}Y_{10}$	4057, 53	3	0, 68	419	50
186	$Mg_{65}Cu_{25}Y_5Gd_5$	4399, 25	4	1, 11	422	51
187	$Mg_{65}Cu_{25}Y_8Gd_2$	4194, 22	4	1, 03	420	52
188	$Mg_{65}Cu_{25}Y_9Gd_1$	4125, 88	4	1, 06	423	49
189	$Mg_{65}Cu_{7.5}Ni_{7.5}Zn_5Ag_5Y_{10}$	4251, 97	6	0, 57	422	**47**
190	$Mg_{65}Y_{10}Cu_{15}Ag_5Pd_5$	4493, 52	5	0, 77	437	59
191	$Mg_{66}Zn_{30}Ca_4$	3726, 14	3	0, 79	351	**52**
192	$Mg_{70}Ca_5Zn_{25}$	3536, 49	3	0, 7	393	**49**
193	$Mg_{71}Zn_{25}Ca_4$	3520, 72	3	0, 71	356	**50**
	Ni-based					
194	$Ni_{39.8}Cu_{5.97}Ti_{15.92}Zr_{27.86}Al_{9.95}Si_{0.5}$	6301, 42	6	2, 32	768	117
195	$Ni_{40}Cu_5Ti_{16.5}Zr_{28.5}Al_{10}$	6324, 97	5	2, 3	763	122

Table 4: Continue of Table 1.

No	Compositions	M, g/mol	n	σ_y, GPa	T_g, K	E, GPa
196	$Ni_{40}Cu_6Ti_{16}Zr_{28}Al_{10}$	6318, 97	5	2, 18	765	111
197	$Ni_{40}Ti_{17}Zr_{28}Al_{10}Cu_5$	6303, 29	5	2, 3	762	134
198	$Ni_{45}Pd_{35}P_{20}$	6985, 38	3	1, 74	610	**90**
199	$Ni_{45}Ti_{20}Zr_{25}Al_{10}$	6148, 96	4	2, 37	773	114
200	$Ni_{49}Fe_{29}P_{14}B_6Si_2$	5050, 15	5	2, 41	694	**124**
201	$Ni_{50}Nb_{50}$	7579, 99	2	2, 26	875	132
202	$Ni_{50}Pd_{30}P_{20}$	6746, 75	3	1, 8	602	**92**
203	$Ni_{52.5}Zr_{20}Nb_{15}Pd_{12.5}$	7629, 73	4	2, 71	861	145
204	$Ni_{53}Nb_{20}Ti_{10}Zr_8Co_6Cu_3$	6721, 58	6	3, 01	846	**157**
205	$Ni_{55}Pd_{25}P_{20}$	6508, 11	3	1, 92	610	**98**
206	$Ni_{55}Zr_{20}Nb_{15}Pd_{10}$	7510, 41	4	2, 71	864	146
207	$Ni_{57.5}Zr_{20}Nb_{15}Pd_{7.5}$	7391, 1	4	2, 72	870	146
208	$Ni_{57}Nb_{35}Fe_3Sn_5$	7358, 33	4	3, 1	886	**160**
209	$Ni_{59.35}Nb_{34.45}Sn_{6.2}$	7420, 08	3	3, 8	882	**190**
210	$Ni_{59.5}Nb_{33.6}Sn_{6.9}$	7433, 01	3	3, 1	881	**159**
211	$Ni_{59}Zr_{16}Ti_{13}Si_3Sn_2Nb_7$	6516, 79	6	3	845	**156**
212	$Ni_{59}Zr_{20}Ti_{16}Si_2Sn_3$	6465, 56	5	2, 7	821	**140**
213	$Ni_{59}Ta_{41}$	10881, 77	2	3, 51	1003	**181**
214	$Ni_{60}Nb_{35}Sn_5$	7366, 88	3	3, 85	885	184
215	$Ni_{60}Nb_{36}Sn_3B_1$	7233, 18	4	3, 3	882	**169**
216	$Ni_{60}Nb_{37}Sn_3$	7315, 27	3	3, 7	895	**186**
217	$Ni_{60}Sn_6(Nb_{0.6}Ta_{0.4})_{34}$	8590, 05	4	3, 58	882	164
218	$Ni_{60}Sn_6(Nb_{0.8}Ta_{0.2})_{34}$	7991, 37	4	3, 5	875	161
219	$Ni_{60}Zr_{20}Nb_{15}Pd_5$	7271, 78	4	2, 75	873	148
220	$Ni_{61}Ta_{39}$	10637, 27	2	3, 35	1002	**174**
221	$Ni_{62.5}Zr_{20}Nb_{15}Pd_{2.5}$	7152, 46	4	2, 81	867	150
	Pd-based					
222	$Pd_{40}Cu_{30}Ni_{10}P_{20}$	7369, 59	4	1, 52	593	98
223	$Pd_{40}Ni_{40}P_{20}$	7224, 01	3	1, 74	590	108
224	$Pd_{60}Cu_{20}P_{20}$	8275, 6	3	1, 7	604	91
225	$Pd_{64}Ni_{16}P_{20}$	8369, 45	3	1, 55	452	92
226	$Pd_{77.5}Cu_6Si_{16.5}$	9092, 24	3	1, 51	646	90
227	$Pd_{80}Si_{20}$	9075, 31	2	1, 34	607	70
	Pt-based					
228	$Pt_{57.5}Cu_{14.7}Ni_{5.3}P_{22.5}$	13159, 1	4	1, 47	508	94, 8
229	$Pt_{60}Cu_{16}Co_2P_{22}$	13520, 71	4	1, 1	506	96
230	$Pt_{60}Ni_{15}P_{25}$	13359, 43	3	1, 4	488	96
231	$Pt_{74.7}Cu_{1.5}Ag_{0.3}P_{18}B_4Si_{1.5}$	15342, 91	6	1, 2	479	96
	Re-based					
232	$Re_{46.4}B_{33.4}Hf_{4.0}Si_{16.2}$	10170, 04	4	4, 5	1109	**227**
233	$Re_{49.7}B_{18.4}Zr_{7.5}Si_{17.4}Nb_{7.0}$	11276, 62	5	5, 83	1273	**271**
	Sr-based					
234	$Sr_{60}Li_5Mg_{15}Zn_{20}$	6964, 28	4	0, 3	331	20
235	$Sr_{20}Ca_{20}Yb_{20}(Li_{0.55}Mg_{0.45})_{20}Zn_{20}$	7617, 66	6	0, 36	319	16
236	$Sr_{20}Ca_{20}Yb_{20}Mg_{20}Zn_{10}Cu_{10}$	7790, 22	6	0, 43	351	**43**
237	$Sr_{20}Ca_{20}Yb_{20}Mg_{20}Zn_{20}$	7808, 66	5	0, 45	353	**44**
	Ti-based					
238	$Ti_{32.8}Zr_{30.2}Ni_{5.3}Cu_9Be_{22.7}$	5412, 57	5	1, 83	611	98
239	$Ti_{40}Zr_{10}Cu_{32}Pd_{14}In_4$	6809, 54	5	1, 79	668	**93**
240	$Ti_{40}Zr_{25}Cu_{12}Ni_3Be_{20}$	5314, 16	5	1, 78	601	94
241	$Ti_{40}Zr_{25}Ni_8Cu_9Be_{18}$	5398, 96	5	1, 81	621	**94**
242	$(Ti_{0.5}Cu_{0.5})_{84}Ni_7Hf_5Zr_3Si_1$	6284, 41	6	2, 25	687	105
243	$Ti_{45}Ni_{15}Cu_{25}Sn_3Be_7Zr_5$	5498, 4	6	2, 48	680	**129**
244	$Ti_{45}Zr_{10}Pd_{10}Cu_{31}Sn_4$	6575, 22	5	1, 97	681	95
245	$Ti_{45}Zr_{20}Be_{30}Cr_5$	4508, 84	4	1, 72	602	105, 6
246	$Ti_{45}Zr_{20}Be_{35}$	4293, 92	3	1, 86	597	96, 8
247	$Ti_{50}Be_{40}Zr_{10}$	3666, 08	3	2, 26	673	**114**
248	$Ti_{50}Cu_{20}Ni_{24}B_1Si_2Sn_3$	5496, 02	6	2, 1	726	110
249	$Ti_{50}Cu_{23}Ni_{20}Sn_7$	5859, 75	4	1, 3	681	**70**
250	$Ti_{50}Cu_{42}Ni_8$	5531, 83	3	2, 01	657	**102**
251	$Ti_{50}Ni_{15}Cu_{25}Sn_3Be_7$	5281, 62	5	2, 17	688	110
	W-based					
252	$W_{46}Ru_{37}B_{17}$	12380, 02	3	5, 6	1149	309
253	$W_{46}Ru_{37}B_{15}Si_2$	12414, 57	4	4, 8	1110	244
254	$W_{45}Ru_{36}B_{17}Hf_2$	12452, 09	4	5, 5	1129	262
255	$W_{30}Fe_{38}B_{25}C_7$	7991, 66	4	4, 85	1048	**235**
256	$W_{30}Fe_{38}B_{22}C_{10}$	7995, 26	4	4, 88	985	**234**
257	$W_{30}Fe_{38}B_{19}C_{13}$	7998, 86	4	4, 91	969	**235**
258	$W_{30}Fe_{38}B_{17}C_{15}$	8001, 26	4	4, 91	968	**235**
	Zr-based					
259	$Zr_{41.25}Ti_{13.75}Ni_{10}Cu_{12.5}Be_{22.5}$	6005, 19	5	1, 93	625	**100**
260	$Zr_{41.2}Ti_{13.8}Ni_{10}Cu_{12.5}Be_{22.5}$	6003, 03	5	2	620	**104**
261	$Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$	5994, 36	5	1, 8	620	101
262	$Zr_{45}Cu_{39.3}Ag_{8.7}Al_7$	7729, 76	4	1, 84	711	94
263	$Zr_{45}Cu_{45}Al_{10}$	7234, 46	3	2, 05	708	**105**
264	$Zr_{46}Cu_{37.6}Ag_{8.4}Al_8$	7707, 58	4	1, 82	703	92
265	$Zr_{46}Cu_{30.14}Ag_{8.36}Al_8Be_{7.5}$	7296, 8	5	2, 1	705	**109**

Table 5: Continue of Table 1.

No	Compositions	M, g/mol	n	σ_y, GPa	T_g, K	E, GPa
266	$Zr_{46}Cu_{46}Al_8$	7335, 27	3	1, 67	715	96
267	$Zr_{46.75}Ti_{8.25}Cu_{7.5}Ni_{10}Be_{27.5}$	5970, 99	5	1, 83	623	100
268	$Zr_{48}Cu_{45}Al_7$	7427, 19	3	1, 9	708	90, 1
269	$Zr_{48}Nb_8Cu_{12}Fe_8Be_{24}$	6547, 61	5	1, 6	658	**84**
270	$Zr_{48}Nb_8Cu_{14}Ni_{12}Be_{18}$	6878, 19	5	2, 03	656	**106**
271	$Zr_{52.25}Cu_{28.5}Ni_{4.75}Al_{9.5}Ta_5$	7292, 81	5	1, 84	684	**96**
272	$Zr_{52.5}Ni_{14.6}Al_{10}Cu_{17.9}Ti_5$	8017, 37	5	1, 91	705	90
273	$Zr_{55}Al_{19}Co_{19}Cu_7$	7094, 52	4	2, 2	733	102
274	$Zr_{55}Cu_{30}Ni_5Al_{10}$	7486, 98	4	1, 82	685	**94**
275	$Zr_{57.5}Nb_5Cu_{15.4}Ni_{12}Al_{10}$	7662, 66	5	1, 58	663	85
276	$Zr_{55}Ti_5Cu_{20}Ni_{10}Al_{10}$	7384, 32	5	1, 63	625	85
277	$Zr_{57}Cu_{20}Al_{10}Ni_8Ag_5$	7749, 39	5	1, 75	668	**92**
278	$Zr_{57}Cu_{20}Al_{10}Ni_8Ti_1Ag_4$	7689, 39	6	1, 65	668	**88**
279	$Zr_{57}Cu_{20}Al_{10}Ni_8Ti_2Ag_3$	7629, 39	6	1, 64	664	**87**
280	$Zr_{57}Cu_{20}Al_{10}Ni_8Ti_3Ag_2$	7569, 39	6	1, 71	662	**91**
281	$Zr_{57}Cu_{20}Al_{10}Ni_8Ti_4Ag_1$	7509, 39	6	1, 58	663	**85**
282	$Zr_{57}Cu_{20}Al_{10}Ni_8Ti_5$	7449, 39	5	1, 49	661	82
283	$Zr_{57}Nb_5Cu_{15.4}Ni_{12.6}Al_{10}$	7652, 26	5	1, 8	687	87
284	$Zr_{57}Ni_8Cu_{20}Al_{10}Ti_5$	7449, 39	5	1, 95	657	**102**
285	$Zr_{59}Cu_{18}Al_{10}Ni_8Ta_5$	8170, 15	5	1, 7	673	**90**
286	$Zr_{60}Fe_5Al_{10}Cu_{25}$	7611, 13	4	1, 64	655	92
287	$Zr_{60}Ni_{25}Al_{15}$	7345, 5	3	1, 79	694	81
288	$Zr_{61.88}Cu_{18}Ni_{10.12}Al_{10}$	7652, 56	4	1, 73	653	80
289	$Zr_{61}Cu_{17.3}Ni_{12.8}Al_{7.9}Sn_1$	7747, 15	5	1, 77	665	**93**
290	$Zr_{61}Ti_2Cu_{25}Al_{12}$	7572, 83	4	1, 63	653	82, 8
291	$Zr_{62}Cu_{15.4}Ni_{12.6}Al_{10}$	7643, 85	4	1, 81	652	80
292	$Zr_{62.5}Fe_5Al_{10}Cu_{22.5}$	7680, 33	4	1, 58	651	88
293	$Zr_{64.13}Cu_{15.75}Ni_{10.12}Al_{10}$	7714, 84	4	1, 69	643	**88**
294	$Zr_{64}Cu_{26}Al_{10}$	7760, 35	3	1, 69	662	**87**
295	$Zr_{65}Al_{10}Ni_{10}Cu_{15}$	7739, 5	4	1, 45	652	83
296	$Zr_{70}Al_8Cu_{13.5}Ni_{8.5}$	7958, 29	4	1, 57	625	**83**