Correlations of equilibrium properties and electronic structure of pure metals

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To explore the possible relationship between $e_{\text{bcp}}$ and equilibrium properties of metals, we further calculated the electronic parameters and equilibrium properties of 24 binary alloys including AB and A:B (or AB$_3$) type alloys (Table S1). A parabolic relationship between bulk modulus and $e_{\text{bcp}}$ for A$_3$B (or AB$_3$) type alloys was obtained as illustrated in Figure S1(a), but not for the AB type alloys, which shows a roughly linear relationship between bulk modulus and $e_{\text{bcp}}$ with a mean squared error of 0.818 (Figure S1(b)). However, no strict correlation between $e_{\text{bcp}}$ and cohesive energy or atomic volume was found.

![Figure S1](image)

Figure S1. The relationship between bulk modulus and $e_{\text{bcp}}$ of (a) A$_3$B (or AB$_3$) type and (b) AB type binary alloys.

| Alloys     | Structure | $e_{\text{bcp}}$ ($e/\text{Å}^3$) | $B$ (GPa)    | $V$ ($\text{Å}^3$) | $E_{\text{coh}}$ (eV) |
|------------|-----------|-------------------------------|--------------|-------------------|------------------------|
| AlFe       | B2        | 0.2652                        | 178.36       | 23.61             | 5.67                   |
| AlNi       | B2        | 0.2351                        | 157.66       | 24.21             | 4.98                   |
| HfRh       | B2        | 0.2175                        | 179.76       | 34.63             | 7.40                   |
| TiNi       | B2        | 0.2255                        | 163.83       | 27.10             | 6.04                   |
| TiTc       | B2        | 0.2727                        | 209.33       | 29.61             | 8.46                   |
| ZnAu       | B2        | 0.1999                        | 115.87       | 32.40             | 2.31                   |
| ZrCo       | B2        | 0.2047                        | 151.31       | 32.04             | 6.98                   |
| ZrOs       | B2        | 0.2548                        | 209.39       | 35.37             | 9.17                   |
| AlFe$_3$   | L1$_2$    | 0.3493                        | 215.49       | 44.72             | 6.17                   |
| AlNi$_3$   | L1$_2$    | 0.3136                        | 179.53       | 45.32             | 5.14                   |
| Compound   | Structure | a (Å) | c (Å) | c/a ratio |
|------------|-----------|-------|-------|-----------|
| Cu3Au L12  | 0.2961    | 141.99| 54.17 | 3.52      |
| HfRh3 L12  | 0.3325    | 223.97| 60.79 | 7.08      |
| NbIr3 L12  | 0.4163    | 314.17| 60.32 | 9.13      |
| NbRu3 L12  | 0.3626    | 267.28| 58.83 | 8.70      |
| VIr3 L12   | 0.4503    | 324.77| 56.23 | 8.65      |
| Zr3Al L12  | 0.2060    | 99.22 | 84.09 | 6.34      |
| Co3Ni D019 | 0.3440    | 237.25| 83.64 | 5.92      |
| CoNi3 D019 | 0.3187    | 209.64| 85.85 | 5.30      |
| HfTi3 D019 | 0.2355    | 114.68| 147.50| 6.45      |
| HfZr3 D019 | 0.2047    | 98.53 | 184.87| 6.90      |
| Mg3Cd D019 | 0.1087    | 40.31 | 175.26| 1.39      |
| MgCd3 D019 | 0.1006    | 44.41 | 175.88| 0.99      |
| ZrNi3 D019 | 0.2821    | 170.85| 105.52| 6.02      |
| ZrTi3 D019 | 0.2255    | 108.23| 149.61| 6.42      |