

LETTERS

Relationship between lattice parameters and the lattice stability of some intermetallic compounds

Using artificial neural network and chemical bond parameters, we investigate some regularity about the lattice constants of intermetallic compounds (belonging to MgCu_2 , MgZn_2 , AuCu_3 or CsCl crystal types, respectively). The lattice constant data of 141 intermetallic compounds have been used as a training set. The atomic radii (Teatum's values), valence electron numbers and Pauling's electronegativity of A, B elements are used as inputs. BP method is used to train a three-layered artificial neural network with $\tanh(x)$ as the transfer function. Cross validation technique is used to test the prediction ability of unknown lattice constants of intermetallic compounds. The results indicate that the averaged prediction error (averaged square root value) is about 0.01 nm. It implies that the lattice constant of intermetallic compound is some function of atomic radii, electronegativities and valence electron numbers of constituent elements.

It is well known that the atoms in intermetallic compounds usually tend to be closely packed. For example, ideal MgCu_2 or MgZn_2 type lattice requires the atomic radius ratio of A, B elements $R_A/R_B = 1.225$, while the ideal AuCu_3 type lattice requires R_A/R_B near 1.0. The real lattices, however, can be formed for atoms A and B within a quite large range of R_A/R_B . Hence it is usually considered that some atoms are "compressed" in lattice formation, i.e. some internal strain occurs. A parameter δ , representing the degree of internal strain, can be obtained by the subtraction of the atomic distances between A-A, B-B and A-B (measured values obtained from experimental lattice data) and the sum of Teatum's atomic radii.

It is meaningful to investigate the relationship between the δ values and the stability of lattices of intermetallic compounds. The formability of a crystal type and the melting type (congruent or incongruent melting, here congruent melting corresponds to higher stability) should be some "indicator" of the degree of stability. It is impossible to find a simple relationship between δ value and the above-mentioned "stability indicators". But some regularity can be found if Δx (electronegativity difference) is concurrently considered. To plot a diagram using δ and Δx as coordinates, the intermetallic compounds of higher stability and that of lower stability distribute in different regions in this diagram. It implies that the charge transfer is a rather important factor affecting the stability. A reasonable explanation is the following: charge transfer changes the atomic radii of elements, making the changed R_A/R_B close to the closest packing requirements. Since the δ value is

based on the unchanged atomic radius data, δ as a single parameter cannot determine the crystal stability. In the lattice of AB_n type intermetallic compounds consisting of larger atom A with lower electronegativity and smaller atoms B with higher electronegativity, it has been found that the radius of atom A decreases significantly while that of B is usually nearly unchanged. So it is possible to estimate the lattice constant of these compounds using the Teatum radius data of B atoms only.

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Preliminary study on ESR method for dating age of Hexian Man

The fossil skull of *Homo erectus hexianensis* was excavated in Longtan Cave, Taodian Village, Hexian County, Anhui Province in 1980^[1]. It is an important event since the fossil skulls of Peking Man, Beijing and Lantian Man, Shaanxi Province were found. The skull of *Homo erectus* was first discovered in South China. The age of Hexian Man has been estimated by different methods. The paleoanthropologists and paleontologists suggested that Hexian Man can compare with the Late Peking Man in age, about 250—300 ka B. P. The ages of U-series dating on fossils are concentrated in 150—160 ka B. P.^[2]. The age of thermoluminescence dating on quartz grains in sediments of Layer 2 in the cave is 200 ka B.P.^[3]

In this note, electron spin resonance (ESR) method was used to date on some fossil animal teeth which were buried together with the fossil skull of Hexian Man. The dating age of the oldest tooth sample is about 300 (299.8) ka B.P.

The major parameters of calculating age are listed in table 1.

Except the parameters mentioned above, the self-absorption factor for enamel for β ray, the attenuation factor for dentine for β ray, the correction factors for water and sediments for β and γ rays are all considered in calculation of dose rate.

The accumulated dose value in table 1 is 909.79 ± 69.89 Gy which was obtained by the best fit of non-linear fitting. The error of the value is only about 7.7%, less than that of linear fitting. The sum of square for the non-linear fitting is only 0.031.

ESR age of fossil tooth is generally obtained by taking the mid-value of early uptake