Editor's Corner

● **MOLE** *noun* 1: An insect-eating burrowing animal of small size living chiefly underground. A mole has no external ears. 2: A small blemish on the human skin, usually of dark color. 3: A massive structure, esp. of stone, set up in the water as a breakwater or pier. 4: The amount of substance of a system that contains as many elementary entities as there are atoms in 0.012 kilogram of carbon 12. The abbreviation for mole is "mol".

The most recent description of the International System of Units (SI) [NBS Special Publication 330 by D. T. Goldman and R. J. Bell, Dec 1981] follows the definition 4 above, with the admonition, "When the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles". It has been traditional in the past in alloy thermodynamics (see, for example, Hultgren's *Selected Values*) to use the unit gram-atom to avoid some of the confusion that may arise in specifying the "elementary entity" required for the mole. Because gram-atom is no longer acceptable with SI, the *Bulletin of Alloy Phase Diagrams* will begin an editorial policy of replacing gram-atom with mole.

Consider integral heats for the intermediate phases (compounds) Al_3Ni_2 and AlNi , the first having five atoms in a formula unit, the second two atoms. If the elementary entity were to be a formula unit of Al_3Ni_2 in the first instance and a formula unit of AlNi in the second, the heat for the first would be more than twice that of the second, instead of slightly smaller when gram-atom is specified. The higher heat would arise from the fact that 2.5 times as many atoms are involved in the formation of the first than the second. Two ways of avoiding this artificial situation would be to rewrite these formulae as $\text{Al}_{0.6}\text{Ni}_{0.4}$ or as $0.2\text{Al}_3\text{Ni}_2$ and as $\text{Al}_{0.5}\text{Ni}_{0.5}$ or as 0.5AlNi . In these ways, the mole refers to the same number of atoms in each "compound", and the heats would be the same as if the unit gram-atom had been used. Another way of arriving at the same result would be to specify the elementary entities as moles of atoms, no matter how the phases were designated. Thus AlNi or βAlNi , or β , or $B2$, or CsCl , or $cI2$, or whatever, could designate this phase whose composition varies from 45 to 69 at.% Ni, and the heats would all be referred to atoms as the elementary entities.

The ambiguities of the use of the mole in thermodynamics of alloys could be avoided if the process to which the heats apply was always specified. In the above example, one might write:

Then the heat, $\Delta H = XX \text{ J/mol}$, refers to $0.2\text{Al}_3\text{Ni}_2$. Another way of explicit clarity is to write:

$$\Delta H_f^\circ (0.2\text{Al}_3\text{Ni}_2, \text{fcc Al, fcc Ni, 1000 K}) = XX \text{ J/mol}$$

For partial heats in alloys, where the components are atoms, the mole would continue to refer to a mole of atoms of the element of the appropriate component of the alloy, and thus is identical to the previous usage of gram-atom.

● We take pleasure in welcoming a new binary category editor in this issue of the *Bulletin*. Dr. J. P. Abriata, of the Centro Atomica Bariloche, Argentina has provided an evaluation for Zr and for the Zr-Nb and Zr-Hf systems. Additional binary evaluations have been provided by the category editors for Ti (Dr. J. Murray), Cu (Dr. D. Laughlin), V (Dr. J. Smith), the rare earths (Dr. K. Gschneidner), and Al (Dr. J. Murray).

● In a provocative article (p 4), Professor Mats Hillert has emphasized one aspect of the utility of numerical calculations of phase diagrams. By carrying out such calculations, the resulting diagrams will automatically obey the various rules for the slopes of phase boundaries, without explicit consideration of these rules.

● In a slight change of style, this issue presents two larger than usual utilization items. The application of phase diagrams to diffusion coatings is discussed by John Manning, and to solar cell research by Kim Mitchell. We would be happy to hear from readers as to whether this format is more useful than the shorter vignettes of earlier issues of the *Bulletin*.

● A number of readers have questioned the continuing use of the cover design of the *Bulletin*. The artist's sketch in the blue box has now been used for seven issues (Vol. 1, No. 1 and 2; Vol. 2, No. 1 to 4; and this issue, Vol. 3, No. 1) and will continue to be used unless one of our readers provides us with a more innovative, or more artistic, or more informative design. This contest ends upon receipt of such a design, and the winning artist will be rewarded by having the artist's signature appear on the design.

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