Discussion of "Legendre Polynomial Expansions of Thermodynamic Properties of Binary Solutions"

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In the paper quoted above enhancements to Legendre polynomial expansions for representing the excess thermodynamic properties of binary solutions are presented. Further, formulae are given for the conversion of the coefficients of simple power series or Redlich-Kister polynomials to Legendre coefficients. This discussion is directed toward these conversion formulae.

Pelton and Bale¹ remark that the conversion between the Redlich-Kister and Legendre coefficients has been given previously by Hillert,² but neglect to mention that Van Tyne, Novotny, and Tarby³ had derived a relationship for the conversion between simple power series and Legendre coefficients over ten years ago.

The relationship which provides for the conversion of the coefficients is given by Van Tyne *et al.*'s Eq. [9], which is rewritten below using the nomenclature of Pelton and Bale for the Legendre coefficients (p) and the power series coefficients (q):

$$p_n = (2n + 1) \cdot \sum_{j=n}^m \left(q_j \cdot \sum_{k=0}^n \frac{B_k}{k + j + 1} \right) \quad [1]$$

In this equation, n refers to the order of the modified Legendre polynomial, m is the order of the power series, and B_k are numeric values unique for each order n (values for B_k can be found in column 2 of Pelton and Bale's¹ Table I).

Consider now the application of Eq. [1] for the evaluation of the Legendre coefficients p_n . For example, when $n = 2$ and $m = 7$, Eq. [1] yields

$$\begin{aligned} p_2 = 5 \left[\left(\frac{1}{3} - \frac{6}{4} + \frac{6}{5} \right) q_2 + \left(\frac{1}{4} - \frac{6}{5} + \frac{6}{6} \right) q_3 \right. \\ \left. + \left(\frac{1}{5} - \frac{6}{6} + \frac{6}{7} \right) q_4 + \left(\frac{1}{6} - \frac{6}{7} + \frac{6}{8} \right) q_5 \right. \\ \left. + \left(\frac{1}{7} - \frac{6}{8} + \frac{6}{9} \right) q_6 + \left(\frac{1}{8} - \frac{6}{9} + \frac{6}{10} \right) q_7 \right] \end{aligned} \quad [2a]$$

which reduces to

$$p_2 = \frac{1}{6} q_2 + \frac{1}{4} q_3 + \frac{2}{7} q_4 + \frac{25}{84} q_5 + \frac{25}{84} q_6 + \frac{7}{24} q_7 \quad [2b]$$

In a similar fashion, when $n = 7$ (and $m = 7$), Eq. [1] may be written as

$$p_7 = 15q_7 \left[-\frac{1}{8} + \frac{56}{9} - \frac{756}{10} + \frac{4200}{11} - \frac{11550}{12} + \frac{16632}{13} - \frac{12012}{14} + \frac{3432}{15} \right] \quad [3a]$$

which yields

$$p_7 = \frac{1}{3432} q_7 \quad [3b]$$

The results shown in Eqs. [2b] and [3b] are identical to the relationships for p_2 and p_7 shown in Pelton and Bale's Table IV.

It is therefore emphasized that the conversion formulae presented by Pelton and Bale in their Table IV for calculation of Legendre coefficients from power series coefficients can all be derived from one equation. Van Tyne *et al.* have noted that a simple computer program can be written which utilizes Eq. [1] to convert the coefficients of a power series into the Legendre coefficients. As a result, solution thermodynamic data which have already been examined and put into a power series representation can be easily converted into a Legendre series representation. If this conversion was more widely known, it might enhance the use of Legendre polynomials by others, a goal sought by Pelton and Bale.

REFERENCES

1. Arthur D. Pelton and Christopher W. Bale: *Metall. Trans. A*, 1986, vol. 17A, pp. 1057-63.
2. M. Hillert: *CALPHAD Journal*, 1980, vol. 4, no. 1, pp. 1-12.
3. C. J. Van Tyne, P. M. Novotny, and S. K. Tarby: *Metall. Trans. B*, 1976, vol. 7B, pp. 299-300.

Authors' Reply

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We were indeed aware of Dr. Tarby's earlier paper. Due to an oversight on our part we neglected to make reference to it. We fully agree with everything he says in his discussion.

Pulsed Laser Control of Surface Solidification

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In a recent paper¹ we were able to show theoretically that the study of solidification parameters during the initial transient during surface melting with a moving heat source gave rise to unique heat flow situations. This was demonstrated

*ARTHUR D. PELTON and CHRISTOPHER W. BALE: *Metall. Trans. A*, 1986, vol. 17A, pp. 1057-63.

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