CONTRIBUTION TO THE STUDY OF THE ORDERING OF THE SIGMA PHASES (*)

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ABSTRACT — Polyhedra around the atomic sites of the sigma phase structure were defined in a way similar to Wigner-Seitz cell and computer programs for the calculation of their volumes were written; the apllication to the sigma phase Mo_3Co_2 shows that again the J-sites exhibit a peculiar behaviour.

The ordering of sigma phases has been discussed in terms of two determining factors: electronic configuration, and size of constituent atoms [1], [2]. Recent work [3] shows that a sphere-packing model is not appropriate and it appears that the occupancy of the J-sites is determined by the electronic factor [4]. As an attempt to obtain more information it was decided to calculate the volume of the polyhedron, around each site, defined in a way similar to the Wigner-Seitz cell.

For the calculation of the volumes of the polyhedra computer programs were written, having the following main steps:

1. Determination of the polyhedra corners.
2. Determination of the intersections of the polyhedra with parallel planes.
3. Calculation of the volumes of the slabs defined by the parallel planes and, from these, the volume of the corresponding polyhedron.

The results obtained for the sigma phase Mo_3Co_2 are listed in Table I.

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The volume of the unit cell calculated by adding the volumes of its 30 polyhedra is 410.4 Å^3, whereas the volume given by unit cell parameters is 411.10 Å^3, which shows an agreement of the order of 0.2 %. Similar calculations will be carried out for other sigma phases and the results will be compared.

TABLE I — Volumes of the polyhedra for the sigma phase Mo_3Co_2

Site	Multiplicity	Occupancy	Coordination number	Polyhedron volume
A	2	2 Co	12	12.38 Å^3
I_1	8	8 Co	12	12.94 Å^3
I_2	8	7 Mo + 1 Co	14	14.42 Å^3
J	8	7 Mo + 1 Co	14	13.53 Å^3
G	4	4 Mo	15	14.63 Å^3

Table I shows that the volume corresponding to the J-site is significantly smaller than that corresponding to I_2, although both have the same coordination number and occupancy. However, J-sites are special sites in the structure, forming linear chains with abnormally short interatomic distances.

REFERENCES

[1] HANSEN, R. C., RAMAN, A., *Z. Metallkd.*, **61**, 115 (1970).
[2] WILSON, C. G., SPOONER, F. J., *Acta Cryst.*, **A29**, 342 (1973).
[3] ALTE DA VEIGA, L. M., COSTA, M. M. R. R., DE ALMEIDA, M. J. M., ANDRADE, L. R., MATOS BEJA, A., *Acta Cryst.*, **A37**, 197 (1981).
[4] ALTE DA VEIGA, L. M., COSTA, M. M. R. R., DE ALMEIDA, M. J. M., ANDRADE, L. R., MATOS BEJA, A., *Acta Cryst.*, **B36**, 1750 (1980).