

Figure 4 Per cent undercooled spheres versus sphere diameter or sphere volume, VM300 maraging steel atomized in argon.

rate. It has not been possible to establish a definite pattern. One of the basic difficulties in following this approach appeared to be the

dependence on cooling rate or sphere size of the modification of the initial solute concentration profile, no matter how small.

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T. Z. KATTAMIS  
 Department of Metallurgy,  
 University of Connecticut,  
 Storrs, Connecticut, USA

R. MEHRABIAN  
 Department of Metallurgy and Materials Science,  
 Massachusetts Institute of Technology,  
 Cambridge, Massachusetts, USA

**Polymorphic transformation NaCl ⇌ CsCl type: additional structural correspondence**

The way in which the CsCl and NaCl structures interconvert in polymorphic MX compounds may be a guide to probable displacements in other structure changes since important structures such as fluorite are geometrically related to these. In investigations of CsCl and ammonium halides the orientation relation  $(001)_{NaCl} \parallel (001)_{CsCl}$ ,  $[110]_{NaCl} \parallel [100]_{CsCl}$ ,

or an orientation  $5^\circ$  from it, has been observed among others [1-4]. This was the only orientation relation between NaCl- and CsCl-related forms of  $RbNO_3$ , though there the geometry is complicated by an intermediate rhombohedral phase [5, 6]. The NaCl arrangement can be converted to the CsCl by a strain having the common  $\langle 111 \rangle$  as principal axis [7, 8]. Martensite computations based on the  $\langle 111 \rangle$  strain accounted for the other orientations, and the shape changes, at large supercooling, but not this orientation [9]. It could be obtained by

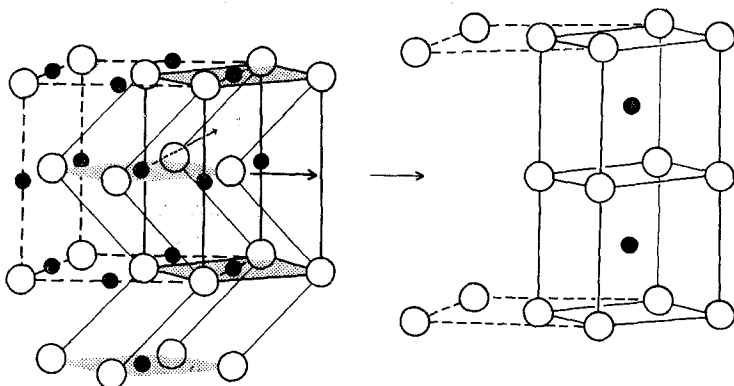


Figure 1 Conversion of the NaCl to the CsCl structure by "unfolding" of the packing and separation of cation and anion layers parallel to (001). Alternate (001) layers translate as indicated and the interlayer spacing of like ions increases. The outlined tetragonal cell becomes two CsCl cells.

successive twinning involving several different  $\langle 111 \rangle$  options but only as a secondary effect [3]. The following additional structural correspondence leads directly to this type of orientation relation.

In the NaCl structure as shown in Fig. 1, the (001) nets (shaded) contract uniformly to conform to the dimensions of the CsCl phase. Simultaneously, alternate layers of X ions translate relatively through  $a/2$ , while in conformity with the contraction of these nets the M ions are displaced into positions between them. An accompanying adjustment of the spacing along [001] gives the CsCl structure in the required orientation. To emphasize that this is physically feasible the reverse change may be regarded as coalescence of the (001) layers of M and of X in CsCl. This would place like ions directly above one another in successive layers, which would translate relatively to avoid such close approach. In this deformation as in the  $\langle 111 \rangle$  strain, the ions pass to their new positions without any activated jump. For CsCl itself,  $a_{\text{NaCl}} = 7.07 \text{ \AA}$ ,  $a_{\text{CsCl}} = 4.22 \text{ \AA}$ ,  $\Delta V/V_{\text{NaCl}} = 0.15$ . The principal distortions (length in product/length in parent) for  $\text{NaCl} \rightarrow \text{CsCl}$  phase are

$$\begin{aligned} [001] \text{ strain } \eta_3 &= 1.19 \quad \eta_1 = \eta_2 = 0.84 \\ [111] \text{ strain } \eta_3 &= 0.59 \quad \eta_1 = \eta_2 = 1.19. \end{aligned}$$

The [001] strain requires smaller deformations. A deformation requiring the minimum changes of length may cause less rapid build-up of misregistry and has been preferred for a martensitic mechanism [10].

There are three options for the unique strain axis, parallel to any cube axis. Pairs of options could produce transformation twinning on  $\{111\}_{\text{CsCl}}$  derived from  $\{110\}_{\text{NaCl}}$ , where CsCl structure is the product. Martensite computations by Fraser and Kennedy (unpublished) show that these twinning modes, and also expected slip modes, do not accommodate the misregistry.

Transformations might, however, show structural control of orientation without being martensitic. Kennedy and Schultz [11] suggested that in thermally activated transformations

micro-regions may be transferred to the product phase non-diffusively perhaps by a dislocation mechanism. Present consideration of deformations to interconvert crystal structures of compounds shows how the micro-regions containing many atoms could transform homogeneously. The activated process would be the release of stress and misregistry by diffusive mechanisms including dislocation climb. These micro-blocks could account for the unpredicted high rates observed for thermally activated advance of a phase interface ([11] and references therein). In the structural transformation  $\text{CsCl} \rightleftharpoons \text{NaCl}$  type the observations suggest that the  $\langle 111 \rangle$  and  $\langle 001 \rangle$  strains both operate.

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S. W. KENNEDY  
Physical and Inorganic Chemistry Department,  
University of Adelaide,  
Adelaide, Australia