

CONCLUDING REMARKS

The consideration of the process of formation of the chemical compound layers in binary heterogeneous systems, carried out in this book, is actually based upon the two simple and obvious assumptions:

- (1) About the quasistationary distribution of the concentration of the components in all the phases involved into the interaction.
- (2) About the summation of the time of lattice diffusion and that of subsequent chemical transformations in the solid-state growth of chemical compound layers.

When combined with the very fundamental concepts and laws of chemistry and physics, these allow the kinetic dependences most often observed experimentally to be derived from a single viewpoint. Clearly, not all the details of the experimental dependences may be unambiguously interpreted on the basis of the proposed relations, the more so that in analysing the mathematical equations attention was only paid to apparent limiting cases. No doubt, this reduced the number of dependences which could be obtained from the same premises without additional assumptions.

Nevertheless, in this book the number of the theoretically substantiated kinetic equations, for the experimentalist to use in practice, appears to exceed that resulting from purely diffusional considerations. Whether the experimentalist will be pleased with such an abundance of equations is a wholly different question. It is so tempting to employ the only parabolic relation and then to discuss in detail the reasons for (unavoidable and predictable) deviations from its course...

Of possible directions of further experimental work, the following are worth mentioning.

- (1) Accumulating the data on reaction kinetics for a variety of chemical compounds under well defined conditions on a systematic basis. It should be recognised that, in spite of a number of investigations which have been and are being carried out in the field, the available experimental data bear an odd character. In most cases, their juxtaposition and theoretical treatment is hardly possible.
- (2) Thorough experimental check of basic kinetic equations in order to verify the existing theoretical views. This applies, for example, to equations of the type (1.64) and (1.65). Although the possibility of growth of the layers of chemical compounds without any homogeneity range is no longer questionable, a relationship between the reaction-diffusion coefficient of a component in the growing compound and the self-diffusion

coefficient of the same component in the non-growing one cannot still be regarded as unambiguously established. It may turn out that equations (1.64) and (1.65) are only the landmarks indicating the way to a solution of this problem rather than the solution itself.

The main obstacle to performing systematic detailed studies likely to provide an insight into the underlying chemical and physical phenomena appears to be the economical pressure for a marketable product, device or technology to pay for the research. Unfortunately, even scientific funds refuse to support pure science, though often readily finance projects without any serious substantiation, containing (mostly unrealistic) promises to make a revolution in production or technology. The present scattered and poorly coordinated approach can scarcely produce scientific results of considerable value. Rather, these are likely to be incommensurably small when juxtaposed to expenditures.

As to theory, attention is to be directed towards

- (1) Establishing the relationships or at least correlations between the values of the chemical and physical (diffusional) constants on the one hand, and the physical-chemical properties of the compounds and their components on the other.
- (2) Mathematical analysis of kinetic dependences, especially in the vicinity of the critical values of the layer thicknesses.

It should be emphasised that of primary interest for both theory and practice is the investigation of the very beginning of interaction of initial substances, including the linear region of growth of compound layers, which has still been explored insufficiently well.

I hope that the reader have understood how dangerous it is to ignore any of the two steps of the reaction-diffusion process (either reaction or diffusion). Irrespective of his educational basis, the researcher must realise that only chemistry, physics and mathematics, taken together, even in the rather moderate amount, are likely to result in the correct consideration of solid-state chemical kinetics. That the physicist never learned chemistry, while the chemist may be unaware of Fick's laws, is not a sufficient reason for the former to ignore the step of reaction or for the latter to do the same with the step of diffusion. Attention is to be paid to secondary and accompanying effects as well, but of course not at the expense of the main features of the process. Continuous interplay of theory and experiment is essential in order that not to conduct fruitless experiments and not to put forward misleading theories.

It appears relevant to note that many workers tend to overestimate the significance of thermodynamic predictions concerning the direction of the reaction-diffusion process. In fact, however, those only bear a likelihood character. Even if the free energy of formation of one compound is -200 kJ mol^{-1} , while that of the other is -20 kJ mol^{-1} , this does not necessarily mean that the former will occur first and the more so that its growth rate must be ten times greater than that of the latter. As exemplified with the growth rate of a compound layer in various diffusion couples of the same multiphase binary system, the opposite may well take place. Categorical judgements must be avoided even in cases of a positive change in the free energy of formation of a compound. Account is to be taken of other chemical reactions proceeding simultaneously, because it may happen that the loss of energy in one of them is offset by its gain in the other(s), thus making the former possible.

It remains to me to express my hope that the reader has convinced that, starting from physicochemical views, it is indeed possible to derive a self-consistent and rather accurate description of the experimentally observed compound layer-growth kinetics. At least, most probable types of the layer thickness-time dependence can readily be predicted. Also, in some (very limited as yet) number of cases it is even possible to precisely calculate the parameters of theoretical equations governing the process of layer growth.