Preface

This volume of Diffusion Foundations is devoted to diffusion and charge transport in bulk and nano-materials. One chapter considers thermal transport in sedimentary materials of the earth crust. The volume consists of an application-oriented one (chapter 1), two theoretical (chapters 2 and 3), three experimental papers (chapters 4 to 6).

Chapter 1 by V. Döge and A.W. Imre with the title 'Charge Transport in Energy Storage and Conversion Devices' is an application-oriented paper. Charge transport by ions is one of the most important phenomena, which directly influences the performance of energy storage and conversation devices. The authors provide an overview of various rechargeable energy storage battery chemistries and designs. They discuss the charge transport processes related to the power capability of the lithium-ion technology. The power-capability, specific energy, and energy density of the industry-relevant Li-ion battery cells based on the electrical loss time approach are summarized.

Chapter 2 presented by L. Momenzadeh, B. Moghtaderi, X. Liu, Scott W. Sloan, I. V. Belova and G.E. Murch has the title 'The Thermal Conductivity of Magnesite, Dolomite and Calcite as determined by Molecular Dynamics Simulation'. Most sedimentary rocks are carbonates which are widely distributed in the earth's crust. Calcite, dolomite, magnesite, and siderite are the most common carbonate minerals. In this study, the phonon-based thermal conductivity of magnesite (MgCO3) and dolomite (CaMg(CO3)2) is calculated and compared with a recent calculation on calcite (CaCO3). Molecular dynamics simulation by way of the Green-Kubo formalism is used for calculating the thermal conductivity. Finally, this chapter provides a comparison of the thermal conductivity from this study and experimental data.

Chapter 3 by F. Hergemöller and N.A. Stolwijk has the title 'Monte Carlo Simulation of Correlation Effects in a Random sc Alloy via Interstitialcy Mechanisms'. In this paper recent progress in the area of Monte Carlo simulation of diffusion via the interstitialcy mechanism in a randomly ordered binary alloy is reviewed. Topics discussed include the calculation of tracer correlation factors as a function of composition and jump frequency ratio and interstitialcy correlation factors. The latter play a crucial role in the interpretation of ion-conductivity data. Diffusion and ionic conduction by the interstitialcy diffusion mechanism in a simple cubic random AB alloy was analysed in the limit of low interstitialcy concentration.

Chapter 4 by G. S. Collins has the title 'Diffusion and Equilibration of Site-preferences following Transmutation of Tracer Atoms'. This chapter describes studies of diffusional nuclear relaxation of the quadrupole interaction at nuclei of Perturbed Angular Correlation (PAC) probe atoms with the aim to determine jump-frequencies and their systematics. These studies were carried out on series of rare-earth indides and palladides having the L12 structure in order to measure diffusional nuclear relaxation of the quadrupole interaction at nuclei of PAC probe atoms. The aim is to determine jump-frequencies and their systematics.

Chapter 5 by Le Zhou and Yongho Sohn is devoted to 'Diffusion and its Application in NiMnGa Alloys'. Heusler NiMnGa alloys are often categorized as ferromagnetic shape memory alloys or magnetocaloric materials. The NiMnGa alloys undergo a series of diffusion-controlled and diffusionless transformations from high temperature to low temperature. Among these transformations the martensitic transformation from an austenitic phase to martensitic phase is critical in determining the properties of the alloys. Although martensitic transformations are considered diffusionless, diffusion also has important applications in the research of NiMnGa alloys. In this paper diffusion couples have been used to study the ternary phase diagram in NiMnGa alloys. The diffusion coefficients provide useful information for fabricating NiMnGa alloys through diffusional processes. The results demonstrate the capability of using diffusion couples to speed up the discovery of new NiMnGa alloys or other alloys showing martensitic transformation.

Chapter 6 by J. Kärger and R. Valiullin has the title 'Transport-Optimized Nanoporous Materials for Mass Separation and Conversion as Designed by Microscopic Diffusion Measurement'. Nanoporous materials find widespread application in material upgrading by separation ("molecular sieving") and catalytic conversion. Mass transfer in these materials is a key phenomenon deciding about their technological performance. This chapter deals with the application of measurement techniques which are able to follow the diffusive fluxes of the guest molecules in nanoporous materials over "microscopic" distances. These techniques include the Pulsed Field Gradient (PFG) technique of Nuclear Magnetic Resonance (NMR) and the techniques of microimaging by interference microscopy (IFM) and by Infrared Microscopy (IRM). The techniques of "microscopic" measurement are able to cover transport phenomena over fractions up to tens of micrometers. In this way details of mass transfer, such as the rate of intra-crystalline diffusion or of the permeation through transport resistances on the surface of the individual crystallites, become accessible by direct experimental observation.

H. Mehrer

The two volumes of Diffusion Foundations with the titles ***Diffusion in High-Tech Materials*** and ***Diffusion and Thermal Transport in Bulk and Nano-Materials*** are dedicated to the memory of Professor Dr. Nicolaas Augustinus Stolwijk

Nicolaas Augustinus Stolwijk, also called Nico by his friends, died suddenly and unexpectedly on May 22, 2017 at the age of 66 in his home near Münster, Germany. This was a shock for his wife Petra, his daughters Judith and Miriam, and his son Sebastian with family. Many friends from the diffusion community including myself, were deeply affected as well.

The diffusion community has lost a person with great merits in diffusion science. Nico performed studies, which covered a wide spectrum of diffusion processes. He studied diffusion in metals, in intermetallic compounds, in semiconductors, in solar grade silicon, diffusion and electrolytic conduction in polymer electrolytes, and diffusion in minerals. He also served the diffusion community as co-organizer of DIMAT 1996 in Nordkirchen near Münster and as organizer of DIMAT 2014 in Münster. During DIMAT 2017 in Haifa, Nico presented two remarkable papers. One week after he returned from Haifa to his home he passed away.

Nicolaas Augustinus Stolwijk was born in 1950 at Gouda in the Netherlands. He started to study physics in Utrecht already at the age of 17. He worked for his PhD in the group of Professor Hans Bakker at the University of Amsterdam. The topic of his PhD work was diffusion in the intermetallic compound cobalt-gallium. As a postdoc with an Alexander von Humboldt grant, Nico joined my diffusion group at the University of Stuttgart and started work on diffusion in semiconductors. In 1984 I received the chair and director position of the Institut für Materialphysik at the Physics Department of the University of Münster. Nico joined our group and received a permanent position as staff scientist. He got his Habilitation at the University of Kiel in 2001 and in Münster in 2005 with his research on 'Diffusion Behaviour and Electrical Properties of Point Defects in Semiconducting Elements, Alloys, and Compounds'. He became Professor in Münster at 2008. Nico was an invaluable support for the institute. He continued to work in this position after my retirement in 2006. He had successfully established a group of PhD and master students. In his group, about 27 PhD and master students performed diffusion studies in various materials and finished their thesis. Nico published 165 papers in peer-reviewed international journals and scientific articles in several books before he retired in 2015. Even after his retirement he guided several students who finished their thesis in his group.

Nicolaas Augustinus Stolwijk was a remarkable scientist and we will keep him in mind as a very likeable colleague and friend with an always supportive and positive attitude. Nico and I were good friends. We published more than 40 common papers on diffusion and point defects in semiconductors and many further papers on diffusion in metals.

Helmut Mehrer

Retired Professor and Director of Institut für Materialphysik, University of Münster, Germany