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James W. Mayer and James K. Hirvonen

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Modern technology depends on materials with precisely controlled properties. Ion beams are a favored method to achieve controlled modification of surface and near-surface regions. In every integrated circuit production line, for example, there are ion implantation systems. In addition to integrated circuit technology, ion beams are used to modify the mechanical, tribological, and chemical properties of metal, intermetallic, and ceramic materials without altering their bulk properties. Ion–solid interactions are the foundation that underlies the broad application of ion beams to the modification of materials. This text is designed to cover the fundamentals and applications of ion–solid interactions and is aimed at graduate students and researchers interested in electronic devices, surface engineering, reactor and nuclear engineering, and material science issues associated with metastable phase synthesis.

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**ION-SOLID INTERACTIONS:
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MICHAEL NASTASI

Materials Science and Technology Division

Los Alamos National Laboratory

Los Alamos, NM 87545

JAMES W. MAYER

Center for Solid State Science

Arizona State University

Tempe, AZ 85287

AND

JAMES K. HIRVONEN

Materials Directorate

US Army Research Laboratory

Watertown, MA 02172



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Symbols

a_0	Bohr radius of the hydrogen atom, Eq. (1.15)
a_B	Bohr screening length, Eq. (2.45)
a_c	lattice parameter, Eq. (1.1)
a_F	Firsov screening length, Eq. (2.46)
a_L	Lindhard's screening length, Eq. (2.47)
a_{TF}	Thomas–Fermi screening length, Eq. (2.27)
a_U	universal screening length, Eq. (2.54)
A	mass number, Eq. (1.2)
b	impact parameter, Eq. (3.37b)
c	velocity of light, p. 11
C_d	displacements per unit volume, Eq. (7.35)
C_i	interstitial concentration, pp. 205–8
C_m	power law constant, Eq. (4.56)
C_v	vacancy concentration, pp. 205–8
d	atomic jump distance, Eq. (8.21)
d_c	collision diameter, Eq. (3.54)
d_{hkl}	distance between planes, Appendix A
D	atomic diffusion coefficient, Eq. (8.21)
\tilde{D}	interdiffusion coefficient, Eq. (11.7)
D_{cas}	effective cascade diffusion coefficient, Eq. (11.3)
D_{liq}	liquid interdiffusion coefficient, Eq. (8.34)
D_v	vacancy diffusion coefficient, Eq. (8.23)
e	charge on the electron
E	ion energy

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List of symbols

- E_0 laboratory energy of incident projectile, p. 42
 E_1 laboratory energy of the scattered projectile, p. 42
 E_2 energy of recoil target atom (*see T*), Table 3.1
 E_b binding energy for 1 mole of atoms, Eq. (2.12)
 E_c energy in the center of mass, Eq. (3.16b)
 E_d displacement energy (Section 7.3), p. 143
 E_F Fermi energy, Eq. (2.21)
 E_m elastic modulus, Eq. (2.17)
 E_s dislocation elastic energy, Eq. (12.16)
 E_{ave} average energy deposited per atom, Eq. (13.2)
 E_A^{ion} ion mixing activation energy, p. 319
 E_d^b bulk displacement energy (*see E_d*), p. 392
 E_d^s surface displacement energy, Eq. (13.11)
 E_f^v vacancy formation energy, p. 206
 E_m^v vacancy migration energy, p. 206
 ΔE_{ML} energy loss in one monolayer, Eq. (13.12)
- f_i interstitial correlation factor, p. 205
 f_v vacancy correlation factor, p. 205
 $f(t^{1/2})$ Lindhard's scaling function, Eq. (4.63)
 F force, Eq. (1.10)
 F_D deposited energy, Eq. (7.40)
- $g(\epsilon)$ Lindhard's inelastic energy-loss function, Eq. (7.20)
- h, \hbar Planck's constant, $\hbar = h/2\pi$
 ΔH_{c-a} enthalpy of crystallization, Eq. (12.2)
 ΔH_{coh} cohesive energy, Eq. (11.21)
 ΔH_f heat of fusion, p. 186
 ΔH_{mix} heat of mixing, Eq. (11.8)
 ΔH_{O-D} order-disorder enthalpy, Eq. (12.9)
 ΔH_s heat of sublimation, Eq. (7.2)
- I average excitation energy, Eqs. (5.39), (8.9)
 I_0 ion flux
- J_A atom flux, p. 229
 J_e rate of evaporation, Eq. (9.46)
 J_I ion flux, Eq. (13.7)
 J_r residual gas flux, Eq. (13.6)

List of symbols

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k	Lindhard's reduced electronic stopping factor, Eq. (5.59)
k_B	Boltzmann's constant
K	bulk modulus, Eq. (12.19)
K_d	atomic displacement rate, Eq. (10.12)
K_L	Lindhard's electronic stopping factor (lab units) Eq. (5.58b)
K_n	nuclear stopping factor, Eq. (9.13)
l	angular momentum, Eq. (3.29)
m	power law variable, $1/s$, Eq. (4.55)
m_e	mass of the electron
M	atomic mass (amu)
n_c	coordination number, p. 20
n_e	number of electrons per unit volume, Eq. (5.45)
N	atomic density, atoms/cm ³ , Eq. (1.2)
N_A	Avogadro's number, Eq. (1.2)
N_d	number of displacements, Eq. (7.17)
$N_R(T)$	number of recoils per unit energy, Eq. (7.50)
N_s	average monolayer areal density, atoms/cm ² , Eq. (1.4)
N_d^s	number of surface displacements, Eq. (13.15)
p	particle linear momentum, Eq. (3.29)
$P(E)$	probability of a particle with energy E undergoing a scattering event, Eq. (4.22)
r	radial distance
r_d	displacement production rate, Eq. (7.42)
r_{\min}	distance of closest approach, Eq. (3.38)
r_T	transport cascade radius, Eq. (7.68)
r_0	equilibrium distance, p. 18
R	range, Eq. (5.1)
R_c	radius of curvature for a charged ion in a magnetic field, Eq. (15.1)
R_d	ratio of surface to bulk displacements, Eq. (13.18)
R_i	ion flux/flux of deposited atom, Eq. (13.1)
R_{\max}	maximum range, Eq. (6.37)
R_p	projected range, Eqs. (6.4), (6.29)
ΔR_p	projected range straggling, Eq. (6.30)

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List of symbols

s	power variable in the inverse power potential, Eq. (4.38)
S	stopping cross-section, Eq. (5.3)
S_{cas}	cascade long-range order parameter, Eq. (10.20)
S_{irr}	irradiation long-range order parameter, Eq. (10.15)
S_{LR}	long-range order parameter, Eq. (10.1)
t	dimensionless collision parameter, Eq. (4.62)
t_{q}	quench time, Eq. (7.66)
t_{ML}	thickness of a monolayer
T	energy transferred to struck atom, Eq. (3.25)
T_{e}	epitaxial temperature, p. 390
T_{m}	melting temperature, p. 365
T_{M}	maximum transferred energy, Eq. (3.27)
T_0, T_{s}	substrate temperature, p. 365
ΔT_{S}	spike temperature
U	elastic energy per unit volume, Eq. (12.17)
U_0	surface binding energy, p. 223
v_{atom}	atom velocity, Eq. (3.14)
v_{ion}	ion velocity, Eq. (3.13)
v_0	Bohr velocity in the hydrogen atom, Eq. (1.16)
v_{r}	radial velocity, p. 52
v_{θ}	transverse velocity, p. 51
V_{AB}	ordering energy
V_{c}	Coloumb potential, Eq. (2.4)
V_{D}	volume of disordered material, Eq. (10.16)
V_{I}	individual cascade volume, Eq. (7.71)
$V(r)$	interatomic potential energy, Eq. (2.2)
V_{T}	transport cascade volume, Eq. (7.69)
$W(T')$	fractional damage function, Eq. (7.51)
x	reduced distance, Eq. (2.53)
X_{i}	mole fraction of element i
Y	sputtering yield, Eq. (9.1)
Y_{E}	empirical sputtering yield, Eq. (9.9)
Y_{spike}	spike sputtering yield, Eq. (9.50)

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Z	atomic number
Z^*	charge on an ion, Eq. (5.27)
α	parameter equal to $Z_1 Z_2 e^2$, Eq. (4.10b)
γ	transfer energy efficiency factor, $4M_1 M_2 / (M_1 + M_2)^2$
γ_i	thermodynamic activity coefficient of element i , Eq. (11.12)
Γ_r	distance between two hard-sphere atoms, p. 16
Γ_v	vacancy jump frequency, p. 205
δ_{corr}	correction factor between the transport and individual cascade volumes, Eq. (7.70)
ε	reduced energy, Eq. (3.55)
ε_b	minimum potential energy
ε_s	strain, Eq. (2.17)
η	inelastic energy loss to electrons, p. 153
θ	laboratory angle of the scattered projectile, p. 43
θ_c	center-of-mass angle of the scattered projectile, p. 43
$\bar{\theta}_D$	mean energy deposited in a spike, Eq. (7.67)
θ_{melt}	energy needed to melt a material, Eq. (7.74)
Θ_c	scattering angle, p. 57
λ_m	power law fitting variable, Eq. (4.57)
λ_d	the mean free path between displacement collisions, Eq. (7.56)
Λ	Sigmund's materials factor, Eqs. (9.2), (9.7)
ν	damage energy, Eq. (7.18)
ξ	atomic interaction variable in the damage function, $N_d(E)$, p. 151
ξ_L	Lindhard's electronic stopping correction factor, Eq. (5.57)
ρ	mass density, g/cm^3
ρ_L	reduced length, Eq. (5.11)
σ_s	stress, Eq. (2.17)
σ	total cross-section for a scattering event, Eq. (4.3)
$d\sigma$	differential cross-section, p. 65

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ϕ	laboratory angle of the scattered target atom, p. 43
ϕ_c	center-of-mass angle of the scattered target atom, p. 43
ϕ_i	ion implantation dose, ions/cm ² , p. 119
χ	screening function, Eq. (2.42)
Ψ	angle of incidence in channeling, p. 135
Ψ_k	kinetic barrier to order–disorder transformation, p. 261
Ω_H	heat of mixing parameter, Eq. (11.9)
Ω_v	atomic volume, cm ³ , Eq. (1.3)
$d\Omega$	differential solid angle, p. 64
$\Delta\Omega$	solid angle of detector, Eq. (4.1)

A Solutions Manual providing answers to the Problems sections is available from either Michael Nastasi, Materials Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, or James Mayer, Center for Solid State Science, Arizona State University, Tempe, AZ 85287, USA.

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Preface

Modern technology depends on materials with precisely controlled properties. Ion beams are a favored method – and in integrated circuit technology, the prime method – to achieve controlled modification of surface and near-surface regions. In every integrated circuit production line, for example, there are ion implantation systems. In addition to integrated circuit technology, ion beams are used to modify the mechanical, tribological, and chemical properties of metal, intermetallic, and ceramic materials without altering their bulk properties. Ion–solid interactions are the foundation that underlies the broad application of ion beams to the modification of materials. This textbook is designed to cover the fundamentals and applications of ion–solid interactions.

When we planned to offer an ‘ion implantation’ course at Arizona State University, we were unable to find a suitable textbook. Instead, we developed our own lecture notes, which form the basis of this book. Although intended as a textbook, we believe, on the basis of our own working experience in the field, that it will be a useful reference to professionals who have an interest in ion–solid interactions.

This text is aimed at undergraduate seniors and graduate students interested in electronic devices, surface engineering, reactor and nuclear engineering, and material science issues associated with metastable phase synthesis. The original course was offered by the Department of Materials Engineering. Approximately half of the students came from electrical engineering or disciplines other than materials engineering. Their backgrounds and training varied. Hence, a firm grasp of the underlying concepts of ion–solid interactions in solids needed in the course could not be assumed. For this reason, the first four chapters of the book are devoted to a review of topics on interatomic potentials, binary collisions, and collision cross-sections.

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The purpose of these chapters is to provide a sufficient coverage of the fundamentals for the subsequent chapters.

The remainder of the book is divided into three parts. The first part (Chapters 5 to 9) deals with the analytical descriptions of ion stopping, ranges, radiation damage, and sputtering. Chapter 8 contains a discussion of Monte Carlo and molecular dynamic simulations. These are calculation techniques that play an increasingly important role in the description of ion–solid interactions. The second part (Chapters 10 to 13) is about the materials-related ion beam issues, including ion implantation metallurgy, ion mixing, phase transformations, and film growth. In the third part (Chapters 14 and 15), we deal with issues of industrial applications and ion beam hardware. Since ion implantation into integrated circuits is a highly specialized topic, we do not deal directly with it. Specific references which treat the technology of this topic are given in the Suggested reading section of Chapter 14.

In writing this book, we have benefited immensely from the help of our students in our classes. Their inquiries and responses to our lectures have strengthened the contents and organization of the book. We also owe a debt of gratitude to our many colleagues for discussion and comments. We especially would like to thank Don Rej for his contributions to the section on plasma source ion implantation in Chapter 15. We would also like to thank John Davis of McMaster University, who served as both guest lecturer in our class and advisor. We are grateful to Robert Averback for helpful discussions in the areas of radiation damage and molecular dynamic simulations, to S. S. Lau and Y-T. Cheng for their discussions in the area of ion beam mixing, and to Don Parkin of Los Alamos National Laboratory for discussions on damage effects in polyatomic materials and his general encouragement and support during the course of this project. The superb typing of the manuscript by Ms Linda Woods is sincerely acknowledged. We also thank Robert Cahn, our editor in the Cambridge Solid State Science Series, for his persistence and patience, and Simon Capelin, Philip Meyler, Fiona Thomson and Irene Pizzie of Cambridge University Press for all their assistance and help. Partial support for the writing of this book was provided for by the US Department of Energy, Office of Basic Energy Research, and the National Science Foundation.

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‘ . . . and he said come to the temple and cleanse yourself for the *ion
beam is good.*’

From *The Temple of the Ion Beam*, lyrics and music by
B. Manfred Ullrich and Gerry Garcia, published by
Böhmische Records, Ithaca, New York.