Reprinted from

COMPUTATIONAL
MATERIALS
SCIENCE

Computational Materials Science 5 (1996) 12–16

Anisotropic creep modelling of the single crystal superalloy SRR99

A. Bertram [a], J. Olschewski [b]

[a] *Otto-von-Guericke-University, JFME, D-39106 Magdeburg, Germany*
[b] *Federal Institute for Materials Research and Testing (BAM V.31) D-12200 Berlin, Germany*

Received 15 July 1995; accepted 31 August 1995

ELSEVIER

COMPUTATIONAL MATERIALS SCIENCE

AIMS AND SCOPE

COMPUTATIONAL MATERIALS SCIENCE aims to enhance the communication between experimental materials research and computational work on both existing and new, advanced materials and their applications. It publishes articles of interest to physicists, chemists and materials researchers and engineers and to other scientists involved with materials phenomena and computational modelling. The journal covers computational modelling of materials properties and phenomena, ranging from the synthesis, characterisation and processing of materials, structures and devices to the numerical methodology of materials simulations.

COMPUTATIONAL MATERIALS SCIENCE invites contributions on quantum, classical and statistical mechanical studies, such as, but not limited to: semi-empirical, e.g. tight-binding and embedded-atom methods; first-principle calculations; density-functional theory; atomic and molecular-scale simulations, e.g. MC and MD techniques; other modelling techniques using macroscopic input, e.g. FE-methods, and contributions on properties of materials, including electronic, dynamical, transport, mechanical, growth and thermodynamical properties of materials such as metal and alloys, semiconductors, insulators, superconductors, biomaterials, polymers, ceramics and composites in liquid, crystal, amorphous and cluster-like states.

Issue Management

Mail Address: Elsevier Science B.V., P.O. Box 2759, 1000 CT Amsterdam, The Netherlands.
Street Address: Sara Burgerhartstraat 25, 1055 KV Amsterdam, The Netherlands.
Tel: +31-20-4852517; Fax: +31-20-4852319; Telex: 10704 espom nl; E-mail: E.MATHLENER@ELSEVIER.NL

ORDERING INFORMATION

Computational Materials Science (ISSN 0927-0256). The 1996 Program will consist of three volumes. Subscription prices are available upon request from the publisher. Please address all your requests regarding orders and subscription queries to:

ELSEVIER SCIENCE B.V., Journal Department, P.O. Box 211, 1000 AE Amsterdam, The Netherlands,

or to any subscription agent or bookseller.

Subscriptions are accepted on a prepaid basis only and are entered on a calendar year basis. Issues are sent by surface mail except to the following countries where air delivery via SAL is ensured: Argentina, Australia, Brazil, Canada, China, Hong Kong, India, Israel, Japan, Malaysia, Mexico, New Zealand, Pakistan, Singapore, South Africa, South Korea, Taiwan, Thailand, USA. Air mail rates for other countries are available upon request.

Claims for issues not received should be made within six months of publication, if they are to be honoured free of charge.

COVER: Equivalent stress in an embedded cell model with circular rigid fiber ($f = 0.5$) and hardening metal matrix ($E = 100$ GPa, $\varepsilon_0 = 0.1\%$, $\sigma_0 = 100$ MPa, $N = 0.2$) at 3.8% total strain. This is Fig. 15a of the paper by M. Dong and S. Schmauder in this issue, p. 53.

Published bimonthly

Printed in The Netherlands

ELSEVIER

Computational Materials Science 5 (1996) 12–16

COMPUTATIONAL
MATERIALS
SCIENCE

Anisotropic creep modelling of the single crystal superalloy SRR99

A. Bertram [a], J. Olschewski [b]

[a] Otto-von-Guericke-University, JFME, D-39106 Magdeburg, Germany
[b] Federal Institute for Materials Research and Testing (BAM V.31) D-12200 Berlin, Germany

Received 15 July 1995; accepted 31 August 1995

Abstract

The starting point is a uniaxial non-linear rheological model, which performs the essential properties of the uniaxial behaviour under different loadings, such as monotonous and cyclic creep and LCF. A tensorial generalization of the uniaxial differential equations is derived by a projection method, which gives a general three-dimensional model obeying the crystal symmetries. An identification for the single crystal superalloy SRR99 at 760°C has been made for tensile creep tests in different orientations. The model can be used to determine the creep behaviour of structural elements such as bars, torsional shafts or turbine blades.

1. Introduction

The three-dimensional creep behaviour of crystalline materials can be extremely anisotropic. This fact has to be taken into account when modelling such materials. In the literature basically two approaches can be found for the three-dimensional modelling of the creep behaviour by constitutive laws. One approach is to use classes of slip systems and to introduce one-dimensional creep laws on the slip system level. By superposition of the shears in the slip systems a three-dimensional model is obtained which renders the symmetry properties of the corresponding crystal class. The range of applicability of such models, however, is limited to those creep mechanisms that are related to slip systems. Diffusional creep, for instance, is excluded, as are other creep mechanisms (see Refs. [1–3]).

The other approach, which is presently favoured, uses algebraic tools such as tensor function representations and invariant theory. For the modelling of the one-dimensional behavior, a uniaxial rheological model is introduced which describes the behaviour under uniaxial creep tests in one orientation in its primary and secondary creep phase. Its governing differential equations have been generalized to three-dimensional anisotropic equations by means of a projection method which is described in Refs. [4,5]. We will limit our consideration to the primary and secondary creep phases, as little is known about the tertiary creep phase including anisotropic damage evolution.

The disadvantage of such a phenomenological approach, however, is that most of its material constants do not have an a priori physical meaning. The calibration of these constants has been carried out by comparing the experimental data with computer-simulated experiments. For

0927-0256/96/$15.00 © 1996 Elsevier Science B.V. All rights reserved
SSDI 0927-0256(95)00053-4

three-dimensional anisotropic constitutive models a large number of different experiments in different orientations is needed. In practice, however, tests in the high temperature regime are complicated and expensive. Thus the main difficulty of the present project was the calibration of the model by a rather limited amount of experimental data.

As the test data were obtained at a temperature of 760°C, the model has been calibrated for this single temperature and all material constants have to be considered as isothermal ones.

2. One-dimensional material model

The starting point of our constitutive modelling is the rheological four-parameter Burgers model (Fig. 1) which consists of two springs with elasticities C and K and two dampers with viscosities L and D (see Refs. [6,7]). All of these constants are assumed to be positive. The differential equations of the model are

$$\sigma^{\bullet} = (C+K)\varepsilon^{\bullet} - (C/L + C/D + K/L)\sigma + C/D\tau, \qquad (1)$$

$$\tau^{\bullet} = K(\varepsilon^{\bullet} - \sigma/L), \qquad (2)$$

where σ denotes the stress, ε the strain, and τ an internal variable which corresponds to the stress in the spring K. The strong non-linearity of the creep behaviour is described by the stress dependence of the viscosities

$$D = D_0 \exp(-B\sigma), \qquad (3)$$

$$L = L_0 \exp(-B\sigma), \qquad (4)$$

with the (positive) material constants D_0, L_0, and B. Thus, the viscosities remain constant during monotonic creep.

This one-dimensional model contains the five temperature-dependent parameters C, K, D_0, L_0, and B, which have been calibrated by monotonic and cyclic creep tests of the single crystal SRR99 in [0 0 1] orientation. The model can easily be integrated numerically for given loading conditions. Experimental results and model calculations are presented in Refs. [8–11].

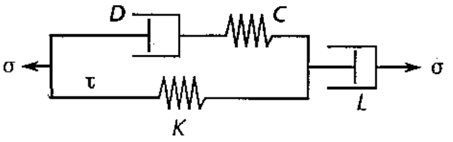

Fig. 1. Rheological Creep Model.

3. Three-dimensional material model

A three-dimensional generalization can be obtained by the projection technique described in Refs. [4,5] in analogy to the elastic behaviour. Hooke's linear elastic law for cubic materials is

$$\boldsymbol{S} = \boldsymbol{C}[\boldsymbol{E}] \qquad (5)$$

where $\boldsymbol{S}$ is the stress tensor, $\boldsymbol{E}$ is the deformation tensor, $\boldsymbol{C}$ is the fourth rank elasticity tensor with cubic symmetry, which can be generally represented as a linear combination in the following form:

$$\boldsymbol{C} = C_1\boldsymbol{P}_1 + C_2\boldsymbol{P}_2 + C_3\boldsymbol{P}_3 \qquad (6)$$

of three independent elastic constants C_1, C_2, C_3 and the three structural tensors

$$\boldsymbol{P}_1 := 1/3\left(\sum_{i=1}^{3} \boldsymbol{e}_i \otimes \boldsymbol{e}^i\right) \otimes \left(\sum_{j=1}^{3} \boldsymbol{e}^j \otimes \boldsymbol{e}_j\right), \qquad (7)$$

$$\boldsymbol{P}_2 := \left(\sum_{i=1}^{3} \boldsymbol{e}_i \otimes \boldsymbol{e}^i \otimes \boldsymbol{e}^i \otimes \boldsymbol{e}_i\right) - \boldsymbol{P}_1, \qquad (8)$$

$$\boldsymbol{P}_3 := \left(\sum_{i,j=1}^{3} \boldsymbol{e}_i \otimes \boldsymbol{e}^j \otimes \boldsymbol{e}^i \otimes \boldsymbol{e}_j\right) - \boldsymbol{P}_1 - \boldsymbol{P}_2, \qquad (9)$$

where $\{\boldsymbol{e}_i\}$ is the lattice base, $\{\boldsymbol{e}^i\}$ its dual, and $\otimes$ the tensor product. By applying the same procedure to the material constants in Eqs. (1), (2) we obtain the tensorial differential equations

$$\boldsymbol{S}^{\bullet} = \boldsymbol{A}_1[\boldsymbol{E}^{\bullet}] + \boldsymbol{A}_2[\boldsymbol{S}] + \boldsymbol{A}_3[\boldsymbol{T}], \qquad (10)$$

$$\boldsymbol{T}^{\bullet} = \boldsymbol{A}_4[\boldsymbol{E}^{\bullet}] + \boldsymbol{A}_5[\boldsymbol{S}], \qquad (11)$$

where $\boldsymbol{T}$ is the tensor of internal variables, $\boldsymbol{A}_i$ are material fourth rank tensors with cubic symmetry, which can be expressed as linear combinations of the three structural tensors $\boldsymbol{P}_i$:

$$\boldsymbol{A}_i = \alpha_{i1}\boldsymbol{P}_1 + \alpha_{i2}\boldsymbol{P}_2 + \alpha_{i3}\boldsymbol{P}_3, \qquad (12)$$

with the scalar coefficients

$$\begin{aligned} \alpha_{1j} &= C_j + K_j, \\ \alpha_{2j} &= -\left(C_j/D_j + C_j/L_j + K_j/L_j\right), \\ \alpha_{3j} &= C_j/D_j, \\ \alpha_{4j} &= C_j/\left(C_j + K_j\right), \\ \alpha_{5j} &= -\alpha_{2j}\alpha_{4j}, \end{aligned} \tag{13}$$

where C_j, D_j, K_j, L_j, $j = 1, 2, 3$ take the part of elasticities and viscosities in different directions. It can be shown that these equations present the complete generalization of Eqs. (1), (2).

As before, the viscosities D_j and L_j depend on the applied stress intensity. In the one-dimensional case there is only one natural stress intensity, but in three dimensions we can define infinitely many. The following ansatz functions, which are based on the cubic integrity base, turned out to be sufficient for our model:

$$D_j = D_{0j} \exp\left(-\sum B_{ij} I_i\right), \tag{14}$$

$$L_j = L_{0j} \exp\left(-\sum B_{ij} I_i\right), \tag{15}$$

with the (positive) material constants B_{ij}, $i = 1, 2, 3, 4$; $j = 1, 2, 3$ and the following cubic scalar invariants (see Ref. [12]):

$$\begin{aligned} I_1 &= \sqrt{\sigma_{xx}\sigma_{yy} + \sigma_{yy}\sigma_{zz} + \sigma_{xx}\sigma_{zz}}, \\ I_2 &= \sigma_{xy}^2 + \sigma_{yz}^2 + \sigma_{xz}^2, \\ I_3 &= \sigma_{xy}\sigma_{yz}\sigma_{zx}, \\ I_4 &= \sigma_{xx}\left(\sigma_{xy}^2 + \sigma_{xz}^2\right) + \sigma_{yy}\left(\sigma_{yx}^2 + \sigma_{yz}^2\right) \\ &\quad + \sigma_{zz}\left(\sigma_{zx}^2 + \sigma_{zy}^2\right). \end{aligned} \tag{16}$$

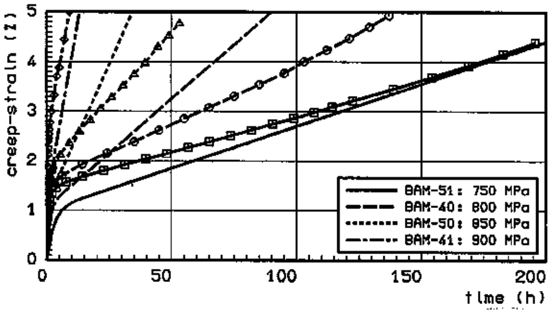

Fig. 2. Identification Tests in ⟨0 0 1⟩-Orientation.

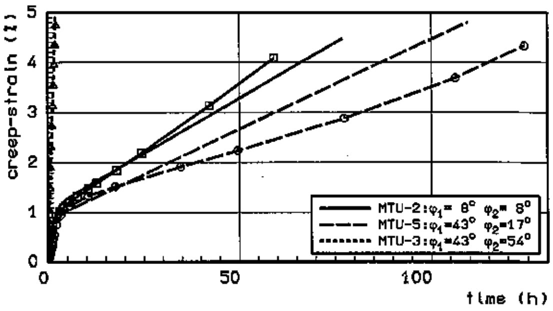

Fig. 3. Identification-Tests at 800 MPa.

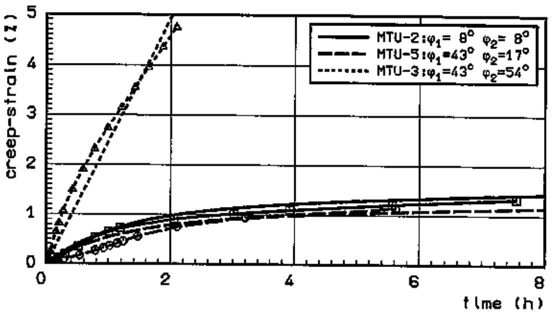

Fig. 4.Identification-Tests at 800 MPa.

The number of material constants can be reduced by the assumption that volume changes occur only elastically. Thus, $D_1^{-1} = L_1^{-1} = 0$ and $B_{i1} = 0$, $i = 1,\ldots,4$.

4. Material identification

The remaining material constants have been identified by tensile creep tests in different orientations for the superalloy SRR99 at 760°C. For that purpose, we divided the experimental data into two groups. The first (identification tests) was used to determine the material constants, the second for comparison of model and experimental behaviour (verification tests). In the diagrams, the symbols represent points of measurement, whereas the curves without symbols have been calculated by the model. φ_i denotes the ith Eulerian angle, determining the orientation of the crystal relative to the specimen. $\varphi_2 = 0$ characterizes the [0 0 1] orientation.

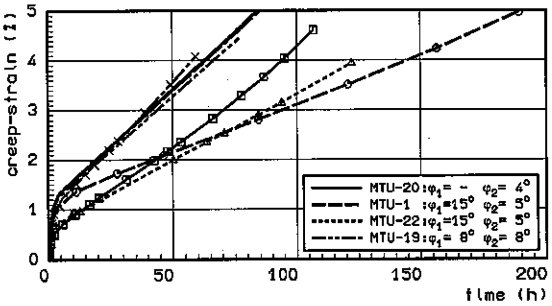

Fig. 5. Verification-Tests at 800 MPa.

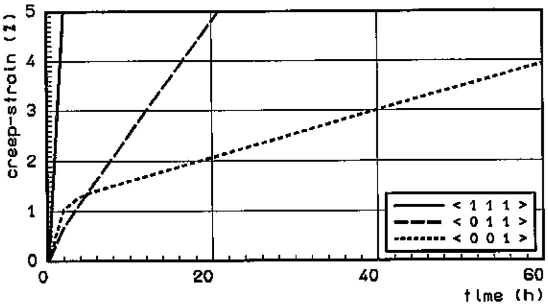

Fig. 7. Calculations at 800 MPa.

The identification tests consists of five tensile creep tests at different stress levels in [0 0 1]-near orientation, performed at the author's institute (Fig. 2), and three tests with different orientations at 800 MPa, performed at Motoren- und Turbinenunion Muenchen (MTU) (Fig. 3, 4). The two diagrams show the same tests with different time-scalings. They demonstrate that the fit gives satisfactory results both in the primary and in the secondary creep phase.

The other tests were used as verification tests (Fig. 5, 6), all of them performed at MTU. It is a common feature of such creep tests that a large scatter band has to be expected. It can be clearly observed from Fig. 6 that specimens with similar orientations under equal conditions can produce rather different creep curves. Accordingly, the calibration of the model should not be overstressed. The agreement of the test and model data turns out to be sufficient if related to the scattering and the limited test data. The model is capable of reproducing the huge difference of the creep strains in different orientations (see Fig. 3). In Fig. 7 the creep curves for the three extreme orientations has been calculated.

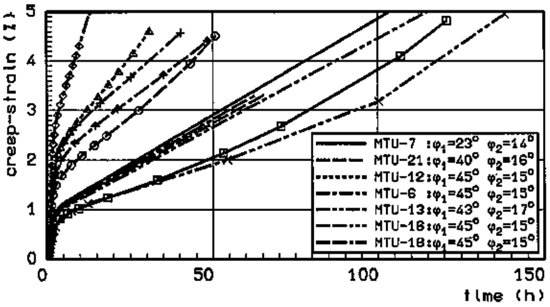

Fig. 6. Verification-Tests at 800 MPa.

The three-dimensional model has been implemented to finite-element codes and used to study the spatial behaviour of torsional shafts with different orientations. Of course, a three-dimensional model requires justification and verification by tests under three-dimensional load conditions such as torsion and combined tension/torsion/pressure tests, which is done by a present project in the field. There are, however, principal problems to be solved for torsional tests on single crystals because of the loss of axial symmetry due to the anisotropy [13,14].

Acknowledgement

This work was funded by Siemens-KWU (Mülheim) within project COST/WP501. The test data were kindly provided by Motoren- und Turbinenunion Muenchen and BAM V.21.

References

[1] J.P. Millour, A. Kobylanski and J. Levy, Acta Metall. 26 (1978) 509–517.

[2] R.A. MacKay and R.D. Maier, Metall. Trans. 134 (1982) 1747–1754.

[3] D.J. Shah, Scr. Metall. 17(8) (1983) 997–1002.

[4] A. Bertram, J. Olschewski, in: High temperature constitutive modeling: theory and application, eds. A. Freed and K.P. Walker (ASME, MD-Vol. 26, AMD-Vol. 121, 1991) p. 129.

[5] A. Bertram and J. Olschewski, ZAMM = Zeit. angew. Math. Mech. 73(4–5) (1993) T401–T403.

[6] N.W. Tschoegl, The Phenomenological Theory of Linear Viscoelastic Behavior (Springer, Berlin, 1989).

[7] G. Backhaus, Deformationsgesetze (Akademie, Berlin, 1983).

[8] A. Bertram, J. Olschewski, M. Zelewski and R. Sievert, in: Creep in Structures, IUTAM Symp., Cracow, Poland, 1990, ed. M. Zyczkowski (Springer, Berlin, 1991) p. 29.

[9] A. Bertram, J. Olschewski, R. Sievert and M. Zelewski, eds. C.S. Desai et al. (ASME, New York, 1991) p. 237.

[10] A. Bertram, in: Berichte des Problemseminars Plastizitätstheorie IV, ed. H. Bergander, 1/91, Technical University Dresden (1991).

[11] A. Bertram, J. Olschewski, R. Sievert and M. Zelewski, Proc. SMIRT-12, Aug. 1993, ed. K. Kussmaul (Elsevier, Amsterdam, 1993) p. 147.

[12] G.F. Smith and E. Kiral, Rend. Circ. Mater. Palermo II (1969).

[13] A. Bertram, J. Olschewski and M. Zelewski, ZAMM = Zeit. angew. Math. Mech. 71(4) (1991) T387–T390.

[14] L. Méric, P. Poubanne and G. Cailletaud, J. Eng. Mater. Technol. Vol. 113 (1991) 162–170.

INSTRUCTIONS TO AUTHORS

Submission of articles should be to one of the Editors (see inside front cover for address).
Format: the journal strives to be accessible to all materials scientists, including those not directly involved in computations. The Editors therefore recommend that articles contain:
1. a self-contained description of the physical problem studied, assumptions used, and results obtained
2. a separate description of the computational method used.

The submission of computational codes in the text of articles is discouraged; the preferred location for these is the electronic bulletin board.
Manuscripts should be typed with double spacing and submitted in triplicate.
The top sheet should contain the title, a running title of at most 45 characters, and the full address, including telephone and fax numbers, of the corresponding author.
Figures should be submitted on separate sheets, drawn in India ink or printed with fine black ink. Lettering of figures should be legible (larger than 1.5 mm) after reduction to one-column size (7 cm).
Colour figures can be reproduced from slides or glossy photographs, at a cost to the author of Dfl. 700 for one page and Dfl. 350 for each consecutive page. A page can contain several figures. These prices are exclusive of Value Added Tax (VAT).
Captions and tables should be given on separate sheets of paper.
References should be numbered in the text and given at the end of the article, e.g.:
for a journal: [1] U. Landman and R. Nieminen, Comput. Mater. Sci. 1 (1992) 10.
for a book: [2] A. Messiah, Quantum Mechanics (North Holland, Amsterdam, 1962) p. 45.
Manuscripts will be refereed; after acceptance and typesetting, **proofs** will be sent by the desk editor (see inside front cover for address) to the corresponding author for correction. Notes added in proof need the consent of one of the Editors.
Copyright should be transferred to Elsevier by means of a copyright transfer form, which will be sent to the author with the proofs.
Reprints: 50 free reprints will be provided for each article, additional reprints can be ordered on a form enclosed with the proofs. Authors of articles containing colour figures receive 200 free reprints.
There are **no page charges** to individuals or institutions.

Submission in electronic form: Articles submitted in electronic form must be accompanied by a set of original figures plus a hard copy of the manuscript.

VIDEO LIBRARY

Videos of simulations illustrative to the research presented in a journal article are welcomed. The video should supplement and illustrate the research described in a scientific paper submitted to the journal. Videos must be submitted to the Editor together with the related paper. Detailed instructions for the preparation of videos can be obtained from one of the Editors or the Desk Editor.

ORDERING VIDEOS: for articles with accompanying videos, in the journal the above sign will be printed with the title of the article related to the video. **Video library listings** will be given at the back of the journal and on the electronic bulletin board.
Videos can be **ordered** with one of the Editors, via fax, bitnet or mail. Please specify your full address, the type and carrier frequency of your video system and the method of payment. The cost of each video is **US$60, to be paid in advance**. Each order should be accompanied by a payment, via credit card, cheque, or money order. If the order is accompanied by adequate reimbursement, a copy is made in the required system. After receiving the order and payment, the video is copied in the required standard and sent via SAL or First Class Mail.

THE CMS BULLETIN BOARD

The Center for Scientific Computing in Helsinki offers an archive for depositing and retrieving scientific software and data in condensed matter physics. We encourage all scientists to deposit software and data associated with articles published in the journal on the server. This service is run on a not-for-profit basis and is free of charge. The bulletin board will be accessible via computer networks, and data can be downloaded through "anonymous ftp".

The bulletin board will contain
- programs and subroutines supplied by authors of journal articles
- data, such as structural coordinates or simulated time sequences pertaining to an article published in the journal
- contents of future issues
- items of further interest, including computer info, etc.
- conference calendar.

To receive the list, send an email containing your own address to physics@csc.fi. You will be notified by email how to use it.

For other information contact:
Kari Kankaala, kankaala@csc.fi (internet), kankaala@finfun (bitnet), +358-31-457 2302 (fax).

Handbook on Semiconductors

Completely Revised and Enlarged Edition

Edited by **T.S. Moss**

Volume 4: Device Physics

Volume edited by **C. Hilsum**

©1993 1244 pages Price: Dfl. 625.00 (US $ 357.25)
Set price: Dfl. 1995.00 (US $ 1140.00) ISBN 0-444-88813-6

The first edition of this volume was published 12 years ago. Since many of the devices described in it were invented 20 years or more earlier, it might have been thought that the field had reached maturity. However, the power of semiconductor physics and the ingenuity of device designers has demonstrated to the contrary. Semiconductor devices have changed so markedly in the intervening decade that this volume is effectively a new book in its own right. Less than one-third of the original material remains, and that, naturally, is largely the fundamental physics. The descriptions of devices are unique and original in each case. The basic layout of the volume is unchanged, and most of the original chapter authors have personally made many of the new advances in design and performance which they describe, as well as incorporating overviews of world progress, in both the context of traditional practice and the latest discoveries. There are two new significant changes in this new edition. The progress in the physics of panel electroluminescence no longer justifies an entire chapter. Whereas superlattices have become so significant recently that the last chapter summarises this field, reporting on the latest advances in preparing semiconductor layers on an atomic scale. The volume includes descriptions of all today's important semiconductor devices, at a level appropriate to the physicist or engineer who is not an expert on that particular device.

Contents: Properties of junctions and barriers *(E.H. Rhoderick et al.)*. Bipolar transistors and integrated circuits *(P.A.H. Hart)*. MOS transistors and memories *(H.-M. Müuhlhoff, D.V. McCaughan)*. Charge coupled devices: physics, technology and imaging *(L.J.M. Esser, A.J.P. Theuwissen)*. Microwave sources *(H.W. Thim, J. Turner)*. Microwave receivers *(P.N. Robson)*. Light emitting diodes *(M.H. Pilkuhn, W. Schairer)*. Semiconductor lasers *(H. Kressel, D.E. Ackley)*. Solar cells *(R.H. Bube)*. Infrared detectors *(C.T. Elliott, N.T. Gordon)*. Nuclear radiation detectors *(E.E. Haller, F.S. Goulding)*. Power devices *(Ph. Leturq, P. Rossel)*. Superlattice and novel multilayer devices *(M.J. Kearney, M.J. Kelly)*. Author index. Subject index.

TO ORDER

Contact your regular supplier or:

ELSEVIER SCIENCE B.V.

P.O. Box 211
1000 AE Amsterdam
The Netherlands
Fax: 020-5862580

Customers in the USA and Canada:

ELSEVIER SCIENCE INC.

P.O. Box 882
Madison Square Station
New York, NY 10159, USA
Fax: 212-6333680

No postage will be added to prepaid book orders. Dutch Guilder price(s) quoted applies worldwide. US Dollar price(s) quoted may be subject to exchange rate fluctuations In all other countries the Dutch guilder (Dfl.) price is definitive. Customers in The Netherlands please add 6% BTW. In New York State please add applicable sales tax. All prices are subject to change without prior notice.

NORTH-HOLLAND

(AN IMPRINT OF ELSEVIER SCIENCE B.V.)