Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

Book Reviews

Version of record first published: 24 Sep 2006.

To cite this article: (1993): Book Reviews, Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals, 237:1, 495-502

To link to this article: http://dx.doi.org/10.1080/10587259308030164

Book Reviews†

Electro-Optical Displays, edited by Mohammad A. Karim, Marcel Dekker, Inc., New York, NY, 1992; xiv + 843 pages; ISBN: 0-8247-8695-5; $165.00.

This book is the thirty-third volume in Marcel Dekker's series on Optical Engineering. Noting the interdisciplinary aspects of the subject, the editor seeks to present an approach for integration of the whole field of display technology. The book consists of 20 chapters divided into four parts: Display Fundamentals; Display Systems; Evaluation of Displays; Display Issues. The intended audience presumably consists primarily of engineers and physicists as neither molecular structures nor names are given for any liquid crystal, dye, or polymer under discussion.

Readers of this journal interested in liquid crystal devices will find the part on Display Fundamentals of most interest. Chapter 2 is a review of liquid crystal properties which are relevant to display devices including recent developments in devices involving ferroelectric liquid crystals. Chapter 3 discusses the use of liquid crystal displays in conjunction with microelectronics based on both amorphous and polycrystalline silicon. Subsequent chapters include discussions of liquid crystals in flat panel displays, liquid crystal light valves, and fast liquid crystal modulators. The final chapter discusses application of liquid crystals in automotive and commercial aircraft cockpit displays from a systems perspective.

Physics of Liquid Crystalline Materials, edited by I.-C. Khoo and F. Simoni; guest editors R. Bartolino, L. Fronzoni, and F. Simoni, Gordon and Breach Science Publishers, Philadelphia, 1991; ISBN 2-88124-481-5(case); xx + 549 pages; $50.00.

This book contains the proceedings of the Summer School on the Physics of Liquid Crystals held in Bra, Italy by the Italian National Liquid Crystals Group on October 4–14, 1988. The guest editors were the organizing co-chairs. The book consists of a forward, a list of contributors, a tutorial chapter of introductory remarks (by R. Bartolino), twenty-two chapters and an index. The twenty-two chapters are divided into three sections: "Microscopic Properties," "Collective Phenomena," and "Special Topics." A major aim of the summer school was to introduce the field to young researchers, and many of the chapters are sufficiently tutorial that this aim was accomplished.

†Unsigned book reviews are by the Book Review Editor.

Crystallography in Modern Chemistry, A Resource Book of Crystal Structures by Thomas C. W. Mak and Gong-Du Zhou.; John Wiley and Sons, 1992; ISBN 0-471-54702-6; xiii + 1323 pages; £136.00.

As both the authors' preface and Professor G. A. Jeffrey's forward note, this book is based on lecture notes in a variety of courses ranging from general chemistry to chemical crystallography. The book is essentially a collection of the description of 141 crystal structures, divided—as is much of the activity in structural crystallography, and the typical program of a crystallography meeting—into "Fundamental Structures," "Inorganic Compounds (Main Groups)," "Inorganic Compounds (Transition Elements)," "Organic Compounds," "Organometallic Compounds" and "Inclusion Compounds."

The first chapter, a twenty page summary of the historical development of structural X-ray crystallography, contains an interesting sprinkling of historical anecdotes, summary charts, reprinted sections of original papers and Chinese characters reflecting the authors' origins. I have used similar material in the first lecture of a course in X-ray crystallography, or even an introductory lecture to high school students, and found here a number of very interesting items to supplement my own material. Many readers will find the list of historically significant papers at the end of the chapter very handy, although a much more complete treatment and comprehensive list of references can be found in the recently published *Historical Atlas of Crystallography* ably edited by J. Lima-di-Faria.

The combined current releases of the Cambridge Structural Databases and the Inorganic Structural Database contain over 200,000 crystal structures. To select less than 150 of the "most important," "most significant" or "most representative" is a formidable task, and one sure to evoke some controversy. Every practitioner of structural chemistry in its various forms will have his own favorites, depending on background and personal interests. Yet it is this reviewer's opinion that the choice has generally been quite well made, and I suspect that most of those chosen by the authors would also appear in a poll to determine the "hit parade" of crystal and molecular structures. Chapter 2 is particularly relevant in that regard, containing many "classic" structures—indeed many of those commonly mentioned in general chemistry texts. The additional explanatory notes accompanying the structures should prove helpful to both instructors and students alike.

A typical entry begins with the name, and empirical formula of the compound in question, space group, cell constants and a list of fractional coordinates. These are followed by a crystal structure, in many cases accompanied by a molecular diagram. There is then usually a section headed "Crystal Structure," which may contain a perfunctory historical remark or two, but generally includes a brief description of the crystallographic and chemical aspects of the structure, including relevant symmetry relations, geometric factors, description of packing, coordination sphere, etc. A subsequent "Remarks" section contains more detailed discussion, including a reference to related materials, and the chemical or physical importance of the compound, or family of compounds, in question. It is in these sections that the authors have cleverly woven a great deal of related chemistry into the text. For instance, deformation density is discussed in seven different entries,

including both organic and organometallic compounds, often together with the structures of the classic cases for these studies. Topics such as absolute configuration, topochemistry, polymorphism, quasicrystalline materials, high T_c superconductors, fullerenes, organic conductors, and many others of current and historical interest to chemists and chemical crystallographers are mentioned in the context of the representative studies of these phenomena. Each entry is copiously referenced and the authors have made a truly laudable attempt to bring the importance of each structure up to date by providing a "Note" following the references with all the latest "hot news" on the subject, often through the end of 1991. (Although I can appreciate the patriotic rationale for scattering a bit of Chinese throughout the text, the inclusion of a reference in Chinese (p. 290) requires at least a citation in Chemical Abstracts for the 80% of the population who still can't read Chinese.) There is also a rather useful general bibiliography which precedes a quite inclusive index.

I expect that this book will prove to be a useful reference for the often classic structures presented, as well as some of the relevant discussion and I found it quite enjoyable for browsing as well. There are, however, a number of features which detract from my overall favorable impression. The significance and the rationale for including each entry would have been clearer by beginning with the historical, chemical, physical or biological importance of the compound in question before the formal presentation the crystallographic data. I have a particular aversion to camera ready copy, and in this I apparently justify the authors' "apprehension" in using this format of presentation. Even perhaps granting the economic necessity for producing a 1300 page book in camera ready copy, in these days of sophisticated microcomputer-based word processing, there is no excuse for the many spelling errors, occasionally very uneven line length, etc.

The book contains over 1000 figures, essentially all of which have been taken from the original literature. Unfortunately, a number of these, especially the older ones, suffer from reproduction (i.e. p. 29) and will prove confusing to the uninitiated reader. Others were poorly designed by the authors of the original papers, and unfortunately the current authors have made no effort to redraw the figures or to provide clarifying explanations in the figure captions. One example of this is the comparison of anatase and brookite in Figure 2.14-3. In another case calcite is presented in a mono view; aragonite in a stereo view. There is an inconsistency in labeling these drawings: some are called "stereoview," while others are "stereoscopic views." Also, many of the novices in viewing stereo diagrams, for whom this book apparently is also intended according to the authors, will find that achieving the stereo effect is quite difficult in many of them. The acceptable range of separation distances between left and right views is 49–62 mm, with 56 mm being the ideal value; some are as small as 37 mm (p. 1164), while others as large as 70 mm (p. 388).

There are also some glaring errors and some imprecise chemical terminology. Representative examples: calcium carbide is a source for *acetylene*, not, as is stated, for ethylene (p. 285); the two lowest energy molecular orbitals for XeF_2 (p. 434) are not correct; "In crystalline α-AgI, the I^- ions constitute a comparatively rigid body-centered-cubic lattice" (p. 448) is a confusing description at best; "Mixed-

valent compounds" (p. 457), rather than mixed valence; the "ordinary" form α of glycine is also imprecise nomenclature; it is the dimethylene bridge in [2.2]-paracyclophane which is disordered, not the "ethylene" bridge (p. 850). Hopefully, these errors will be corrected in a subsequent edition to improve upon what basically is an interesting and potentially useful book.

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Computer Simulation of Polymers, Edited by Ryong-Joon Roe (University of Cincinnati). Prentice Hall Advanced Reference Series: Polymer Science and Engineering Series (Series Editor: James E. Mark, University of Cincinnati), Prentice Hall, Inc., Englewood Cliffs, New Jersey, 07632. 1991. xi + 404 pp. incl. Index; $77.00; ISBN 0-13-161480-0.

Coupled with the development of high-resolution computer graphics, the accessibility of powerful, fast, and dedicated computers and supercomputers has transformed studies in computational and theoretical chemistry in recent years. This is particularly so for the field of polymer science, since now for the first time researchers are able to explore the structure, energetics, and dynamics of large polymeric systems using computer simulations. Polymer scientists have responded with an upsurge of new methods and applications spanning a wide range of topics in computational polymer science. So it is indeed timely that the superb book *Computer Simulation of Polymers* was published last year.

As explained by Series Editor J. E. Mark in the Forward, this book is the first in a series aimed at providing authoritative accounts on polymer science and engineering. The papers collected in this book were originally presented as part of a five-day research symposium of the same name, sponsored by the Division of Polymer Chemistry at the American Chemical Society Meeting in Miami Beach, Florida, on September 11–15, 1989.

Let me state at the outset that I highly recommend this book. It should be considered required reading for anyone who currently works or aspires to work in this field. In fact, I believe this may be the case already since this book seems to be among the most frequently cited references in recent articles covering computer simulations of polymers.

The book is divided into 28 chapters, each authored by recognized experts in their respective subject area. The articles cover a wide range of general areas, most notably: (1) simulations of the rheological and conformational properties, the transitions, and the free-volume distributions of polymer liquids and glasses; (2) simulations of diffusion of polymer molecules themselves and of small molecules through polymers; (3) conformational analysis of rigid polymers by molecular mechanics and quantum mechanical calculations; (4) simulations of phase transitional behavior

of liquid-crystalline polymers; (5) modeling of polymers at interfaces using molecular mechanics and Monte Carlo methods; and (6) calculations of phase equilibria and separation in polymer blends. The general methodologies covered in the 28 chapters break down roughly into the following categories: quantum mechanics (1.5), molecular mechanics (1.5), molecular/Brownian/Langevin dynamics (13.5), Monte Carlo methods (6.5), and Other (5), where the fractions denote splitting between categories.

I especially appreciated several unique features of this book. First, every article is preceded by an Abstract which truly captures the essence of the forthcoming article. Second, the end of virtually every article includes a final discussion or summary that recounts the primary findings of the research. Third, each article is amply annotated with references (698 in all) to the literature thus serving as a resource for background and extended reading. Fourth, the book includes a combined author/subject/name index to enable quick access to topics covered and individuals cited in the articles. Fifth, and most notably, every article is written with outstanding craftsmanship. In each chapter, the author(s) has made every effort to introduce the topic to the non-expert reader and to present the material in a technical but comprehensible manner. The Editor and the authors are to be commended for their consideration for the reader as well as their mastery of the subject area. Moreover, the book is handsomely typeset and bound, amply illustrated, and promises to be eye-catching on any book shelf.

Limitations of space permit only a brief synopsis of each chapter here. In Chapter 1, R. L. Jaffe, D. Y. Yoon and A. D. McLean present a thorough *ab initio* analysis of the molecular geometries, conformational energies, and torsional/vibrational potentials for a series of mono- and diphenyl model compounds that represent building blocks for many thermoplastic high-performance polymers. The results, which are sensitive to the choice of basis set and to the degree of inclusion of electron correlation, differ in some cases from those obtained from semiempirical and molecular mechanics (MM) calculations. Detailed results for bisphenol-A-polycarbonate and for poly(*p*-hydroxybenzoic acid) are presented to illustrate the utility of these potential-energy functions for modeling polymers. In Chapter 2, C. Getino, J. Santamaria, J. A. Darsey, and B. G. Sumpter use *ab initio* calculations and molecular dynamics (MD) simulations to study the cis/trans isomerization process in stilbene, a model compound for poly(phenylenevinylene). They provide very interesting discussions of the isomerization lifetimes and the time evolution for intramolecular energy flow. In Chapter 3, A. Anwer, R. Lovell, and A. H. Windle use MM to calculate the conformational energetics for seven compounds of the form Ph—*X*—Ph, with X = —S—, —O—, —CO—, —CH_2—, —$C(CH_3)_2$—, and —$C(CF_3)_2$—, all of which are structural building blocks in many high-performance polymers. The energetics calculations lead to estimates of the polymer's persistence length. The distinction between static (equilibrium) flexibility and dynamic (kinetic) flexibility is explored. Their analysis includes a compilation of previous conformational energy calculations on these moieties. In Chapter 4, D. C. Doherty and A. J. Hopfinger present a lucid MD characterization of the $\beta_0 \rightarrow \alpha_h$ pre-melting phase transition observed in the higher odd-numbered *n*-alkanes. The results, which are elegantly illustrated, demonstrate the existence of selective

cooperativity among the torsion angles. In Chapter 5, J.-P. Ryckaert, I. R. McDonald, and M. L. Klein discuss MD simulations using an all-atom semiflexible model to examine long-chain paraffins representative of Langmuir-Blodgett films, micelles, and biological membranes. A detailed MD analysis of the C_{23} *n*-alkane (tricosane) in its rotator phase R_I produces results in excellent agreement with experiment. In Chapter 6, D. Rigby and R. J. Roe describe a MD simulation study of *n*-alkanes both above and below their T_g. They examine the bond conformational barrier transition rates and the reorientation motion of individual backbone bonds. They find that the activation energy associated with conformational transitions corresponds closely to a single trans-gauche barrier height and is nearly identical for butane and eicosane. In Chapter 7, R. H. Boyd and K. Pant use off-lattice MC techniques to simulate the structure of simple polymeric liquids and glasses at constant pressure. Their discussion of the reptation model for simulating polymer melts is lucid and very informative. They calculate a number of properties, including values of C_p (resolved into its components), the chain dimensions, and the distribution of interstitial free-volume. In Chapter 8, M. F. Sylvester, S. Yip, and A. S. Argon present constant-pressure MD simulations to investigate the structural and dynamic characteristics of a model compound for poly(propylene) both above and below its T_g. Their work suggests that profound structural differences exist between the liquid and glassy state. In Chapter 9, K. F. Mansfield and D. N. Theodorou present a general MC/MM technique for the detailed atomistic simulation of glassy polymers at interfaces. Using poly(propylene) as an example, they make predictions of the internal energy contribution to surface tension, adhesion tension, and the work of adhesion which agree reasonably well with available experimental values. In Chapter 10, M. Murat and G. S. Grest use MD simulations to explore the equilibrium properties of polymeric brushes consisting of linear polymers grafted at one end onto a repulsive surface. Interactions between brushes are also addressed and analyzed in detail.

In Chapter 11, D. B. Adolf and M. D. Ediger use Brownian dynamics in the high friction limit to simulate the local segmental motions of polyisoprene. They find semiquantitative agreement between their calculated correlation times and those observed by NMR measurements. In Chapter 12, K. Kremer and G. S. Grest present extensive MD simulations of an entangled polymer melt that cover the crossover from Rouse dynamics to reptation. In this interesting article, they find that reptation theory describes the chain dynamics very well. They also recommend using highly idealized, coarse-grained, polymer models for such studies to spare CPU time. In Chapter 13, D. Eichinger and D. E. Kranbuehl study the relaxation behavior of polymers using a nonlattice bead-stick model simulated using MC methods. They find that the effects of excluded volume constraints are much stronger on the long internal relaxation times of the chains than on the equilibrium dimensions. In Chapter 14, H. C. Öttinger discusses an improvement of a recently developed algorithm for simulating the Doi-Edwards and Curtiss-Bird models for concentrated polymer solutions and melts in homogeneous flows. The new simulation algorithm provides a powerful tool for investigating complex flow systems and various generalizations of the original Doi-Edwards and Curtiss-Bird models. In Chapter 15, D. Gersappe and M. O. de la Cruz present a novel application of

off-lattice Langevin dynamics simulations to study gel electrophoresis in a periodic gel. Results of their chain-dynamics simulations differ considerably from those predicted by the tube reptation theories. In Chapter 16, R. F. T. Stepto discusses two applications of MC simulations to study the diffusive behavior of polymer chains. The first application provides a quantitative prediction of experimental diffusion coefficients of short polymethylene chains in various solvents. The second application explores modeling the center-of-mass diffusion in real time using MC simulations. In Chapter 17, S. Trohalaki, A. Kloczkowski, and J. E. Mark describe MD simulations used to estimate the diffusion coefficient for small molecular penetrants in polyethylene. The authors provide a clear and concise introduction to gas diffusion through polymers and discuss possible mechanisms for penetrant diffusion. In Chapter 18, C. M. Lastoskie and W. G. Madden present an interesting discussion of Madden's pseudokinetic simulation technique as extended to polymer models in the continuum. They find that the intra- and intermolecular radial distribution functions calculated using the pseudokinetic algorithm agree quantitatively with those obtained from standard simulations. In Chapter 19, J. H. Weiner and J. Gao discuss their MD simulations of model networks for rubber elasticity consisting of tetrafunctional freely rotating chains with nodes at the sites of a diamond lattice. Their analysis suggests that the macroscopic stress in a deformed network may be regarded as arising from the orientation by the deformation of the so-called intrinsic atomic stress systems.

In Chapter 20, D. R. M. Williams and M. Warner present Langevin dynamics simulations to investigate multihairpin dynamics in nematic wormlike main-chain polymer crystals. They show that the decay of n hairpins may be described by a simple system of master equations. In Chapter 21, C. A. Croxton describes an MC-like Iterative Convolution (IC) technique to study the configurational and nematic $\rightarrow$ isotropic phase transition of polynematic phases represented by a semiflexibility-coupled linear sequence of rods. Agreement between results for the IC method and conventional MC approaches is generally good to excellent. In Chapter 22, B. G. Sumpter, D. W. Noid, B. Wunderlich, and S. Z. D. Cheng present a lucid account of their studies of various structural and dynamical properties of polymers in the solid state using MD simulations. Their results provide insight into the structural changes experienced by a polymer while undergoing a crystalline-phase $\rightarrow$ melt-phase transition. Calculations of the temperature-dependent heat capacities and spectra are also presented and analyzed. In Chapter 23, D. H. Reneker and J. Mazur describe a family of crystallographic defects in polyethylene all characterized by a defect loop that encircles one chain. In Chapter 24, N. A. Neuberger and W. L. Mattice apply the rotational isomeric state (RIS) method to calculate the dimensionless correlation coefficient ρ for r^2 and s^2 for the infinite chain using as examples poly(dimethyl siloxane), polyethylene, poly(phosphate), poly(vinylidene fluoride), poly(oxymethylene), polysilane, and poly(dimethylsilane). They find that, as n increases, ρ approaches the value $(5/8)^{1/2}$ predicted by analytical treatments of the idealized freely jointed chain. In Chapter 25, H. Meirovitch uses the scanning simulation method to carry out a systematic study of the tricritical behavior of relatively long self-avoiding walks (SAWs) and trails in 2D and 3D. In Chapter 26, R. C. Lacher and D. W. Sumners present a set of data structures

and algorithms for the calculation of linking numbers in lattice models. In Chapter 27, M. V. Ariyapadi, E. B. Nauman, and J. W. Haus use a continuum model based on a modified form of the Cahn-Hilliard equation to study the time evolution of the phase separation in polymer-polymer systems by spinodal decomposition. In Chapter 28, Y.-B. Ban and J.-D. Kim describe a new method for calculating the liquid-liquid equilibria of polymeric ternary systems involving two polymers and solvent. The method incorporates the "blob" concept of a polymer chain as well as a renormalization scheme from primary blobs to rescaled blobs. Results are presented for polystyrene-polystyrene-cyclohexane mixtures and for PEG-dextran-water mixtures.

In closing, I believe the serious researcher in this field and related fields will find this book indispensable. It will serve as a valuable resource for years to come. Along with the recently published *Computational Modeling of Polymers* (Ed.: J. Bicerano; Marcel Dekker, 1992), this fine book gives testimony to the rapidly expanding field of computational polymer science.

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Radiation Processing of Polymers, edited by A. Singh and J. Silverman, Hanser Publishers, Munich, 1991; distributed by Oxford University Press (U.S.A. and Canada); xvii + 377 pages; ISBN 3-446-15784-0 (Hanser); ISBN 0-19-520914-1 (Oxford); $84.00.

In this volume, the editors seek to expose scientists and engineers to recent developments in the use of ionizing radiation in the processing of polymers. In recent years there have been several commercializations of materials formed by either radiation-induced crosslinking (e.g., heat-shrink polyethylene tubing) or degradation (e.g., polytetrafluoroethylene lubricants and coatings for pots and pans), not to mention radiation sterilization of medical disposables. The book does not deal with the fundamentals of the interaction of radiation with matter, but rather emphasizes the polymer chemistry and science associated with the processing of different classes of polymeric materials. The book consists of 14 chapters; the first three present an overview, a comparison between radiation-induced and chemical crosslinking, and a description of electron accelerators for industrial processing. The final 11 chapters deal with specific topics and classes of materials and their interaction with radiation. Radiation processing of food was deemed outside the scope of the book. The editors have done a good job in assembling a volume of information showing the advantages of radiation processing in a number of important situations.