
CHAPTER 7

Localized Electrons, Holes and Ions

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1. LOCALIZED ELECTRON STATES

The properties of electrons in liquid dielectrics have attracted the attention of experimentalists and theoreticians. This topic is connected with variety of observed effects,

the study of which makes possible not only an understanding of peculiarities of electron behavior in liquids, but also gathering of information on the properties of liquids themselves. The latter is especially important because theoretical

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Branch and Tree Decomposition Techniques for Discrete Optimization

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Abstract This chapter gives a general overview of two emerging techniques for discrete optimization that have footholds in mathematics, computer science, and operations research: branch decompositions and tree decompositions. Branch decompositions and tree decompositions, along with their respective connectivity invariants, branchwidth and treewidth, were first introduced to aid in proving the graph minors theorem, a well-known conjecture (Wagner's [124] conjecture) in graph theory. The algorithmic importance of branch decompositions and tree decompositions for solving \mathcal{NP} -hard problems modelled on graphs was first realized by computer scientists in relation to formulating graph problems in monadic second-order logic. The dynamic programming techniques utilizing branch decompositions and tree decompositions, called branch decomposition- and tree decomposition-based algorithms, fall into a class of algorithms known as fixed-parameter tractable algorithms and have been shown to be effective in a practical setting for \mathcal{NP} -hard problems such as minimum domination, the traveling salesman problem, general minor containment, and frequency assignment problems.

Keywords branchwidth; treewidth; graph algorithms; combinatorial optimization

1. Introduction

The notions of branch decompositions and tree decompositions and their respective connectivity invariants, branchwidth and treewidth, are two emerging techniques for discrete optimization that also encompass the fields of graph theory, computer science, and operations research. The origins of branchwidth and treewidth are deeply rooted in the proof of the graph minors theorem, formally known as Wagner's [124] conjecture. Briefly, the *graph minors theorem* states that in an infinite list of graphs there would exist two graphs H and G such that H is a minor of G . The algorithmic importance of the branch decomposition and tree decomposition was not realized until Courcelle [50] and Arnborg et al. [15] showed that several \mathcal{NP} -hard problems posed in monadic second-order logic can be solved in polynomial time using dynamic programming techniques on input graphs with bounded treewidth or branchwidth. A problem that is \mathcal{NP} -hard implies that as long as it is not proven that $\mathcal{P} = \mathcal{NP}$, we cannot expect to have a polynomial-time algorithm for the problem. These techniques are referred to as tree decomposition-based algorithms and branch decomposition-based algorithms, respectively. Branch decomposition- and tree decomposition-based algorithms are important in discrete optimization because they have

Opportunities for Combinatorial Optimization in Computational Biology

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This is a survey designed for mathematical programming people who do not know molecular biology and want to learn the kinds of combinatorial optimization problems that arise. After a brief introduction to the biology, we present optimization models pertaining to sequencing, evolutionary explanations, structure prediction, and recognition. Additional biology is given in the context of the problems, including some motivation for disease diagnosis and drug discovery. Open problems are cited with an extensive bibliography, and we offer a guide to getting started in this exciting frontier.

Key words: computational biology; combinatorial optimization; global optimization; integer programming; minimum energy; bioinformatics; molecular structure prediction; protein folding; protein alignment; rearrangements, assembly; sequence alignment; SNP; sorting by reversals

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1. Introduction

Although computational biology has been an increasing activity in computer science for more than a decade, it has been only the past few years that optimization models have been developed and analyzed by researchers whose primary background is operations research (OR). The purpose of this survey is to demonstrate the applicability of mathematical programming, from an OR perspective, to these problems in molecular biology.

We begin with some vocabulary, but more, context-dependent biology will be described in each section. This will not be enough biology to develop your own research in this exciting frontier, but it is enough to understand many of the problems and make an informed decision whether to pursue this field. The appendix offers guidance to getting started.

One class of problems involves sequences from one of the following alphabets:

1. Four nucleotides in DNA (one-letter code in bold capital):

{Adenine, Cytosine, Guanine, Thymine}

2. Four nucleotides in RNA (one-letter code in bold capital):

{Adenine, Cytosine, Guanine, Uracil}

3. Twenty amino acid residues in proteins:

Name	Symbol	Name	Symbol
Alanine	A	Leucine	L
Arginine	R	Lysine	K
Asparagine	N	Methionine	M
Aspartic acid	D	Phenylalanine	F
Cysteine	C	Proline	P
Glutamine	Q	Serine	S
Glutamic acid	E	Threonine	T
Glycine	G	Tryptophan	W
Histidine	H	Trysine	Y
Isoleucine	I	Valine	V

From one sequence's information, we would like to recognize or predict structure. From multiple sequences, we would like to compare structures and determine if they are in the same "family." It is believed, with some reservation, that structure determines function, although this issue is still being

Advances in Nanocrystalline Diamond

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1. INTRODUCTION

“Diamond,” first mined in India thousands of years ago, has been known as the “king of gemstones” by the public for its beauty for centuries. It probably will not be long until in the 21st century the same diamond with a different morphological structure will be known as the “king of materials” to engineers and scientists for its extreme properties with their unique combinations and practical use in manufacturing in the form of films and coatings [1, 2]. The extreme material properties of diamond with some potential applications from their unique combinations can be found in some review articles (for example, see K. V. Ravi in [1] and P. Chalker and S. Lande in [2]), and in addition some new areas of applications such as surface acoustic wave (SAW) devices [2, 3], and micro/nanoelectromechanical systems (MEMS and NEMS, respectively) [4–6] have started emerging. In brief, diamond is very hard and least compressible, is optically transparent from the deep ultraviolet (UV) to the far infrared, has the highest known thermal conductivity of all materials at room temperature, has low thermal expansion coefficient at room temperature (0.8×10^{-6} K) that is comparable to that of invar, exhibits low or “negative” electron affinity, and is biologically compatible and very resistant to chemical corrosion [1, 2, 7, 8]. Diamond is much more resistant to

X-rays, γ radiation, UV light, and nuclear radiation than the other semiconductors such as Si and Ge. Also, it is a very good electrical insulator (with room temperature resistivity of $\sim 10^{16}$ Ω cm). However, its resistivity can be changed over the range $10\text{--}10^6$ Ω cm by doping, thus becoming a semiconductor with a wide bandgap of 5.5 eV. The great interest in diamond also comes from its applications in electronic devices as it has very high mobility (about 2000 $\text{cm}^2/\text{V s}$), breakdown field (10 MV/cm), and saturation velocity (about 2.5×10^7 cm/s) compared to other semiconductors [8]. At the same time, there are other diamond related carbon materials that have properties in between those of diamond and graphite. The properties of these hard carbon materials vary, depending on the concentration of sp^3 - (diamond) and sp^2 - (graphite) bonded carbon in the films. A classification of diamond and related materials in terms of their structure, resistivity, and energy gap is given in Table 1. The energy difference between thermodynamically stable graphite and metastable diamond is 0.9 kcal/mole. Nanodiamond is a metastable material with intermediate energy, close to *ta*-C having sp^3 bonds more than 90% [9, 10]. Before progressing further let us discuss diamond and related materials in some more detail.

1.1. Synthetic Diamond

Scarcity and cost of the natural diamond led scientists to find means of making diamond in the laboratory. Although there have been several attempts to synthesize diamond from various sources of carbon since it was discovered to be an allotrope of carbon, two main techniques were invented, both in the 1950s; high pressure and high temperature (HPHT) synthesis [1, 7] and chemical vapor deposition (CVD) synthesis [1, 2]. To date, since its discovery, most of the demands to supply diamond for industrial uses, primarily for material cutting, grinding, and polishing, are met by the HPHT technique. In this technique graphite is subjected to tens of thousands of atmosphere and heated to over 2000 K in the presence of some metal catalyst crystallizing it in diamond. However, this process is intrinsically limited in its ability to cover surfaces in the form of thin film coatings and to produce large sizes. These limitations are overcome by another technique (i.e., CVD synthesis

INVENTORY COST EFFECT OF CONSOLIDATING SEVERAL ONE-WAREHOUSE MULTIRETAILER SYSTEMS

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Consolidation of warehouses is a new trend in global logistics management, and the reduction in order processing and inventory costs is often cited as one of the main motivations. In this note we show that when retailers face constant demand rates and their ordering costs are independent of the warehouse that services them, consolidated systems are *rarely* suboptimal and *always* lead to close-to-optimal inventory replenishment costs. In particular, we prove that using two (one) properly selected warehouses, the systemwide inventory replenishment cost is in the worst case at most 2% (14.75%) more than the optimal.

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Subject classifications: Inventory/production: multi-item/echelon/stage, deterministic. Facilities/equipment planning: location, discrete.

Mathematics: convexity.

Area of review: Manufacturing, Service, and Supply-Chain Operations.

1. INTRODUCTION

Many companies are streamlining their distribution network by consolidating and centralizing their logistics operations. The Strategies 2005 Report prepared by leading food distributors in the United States suggested that warehouse consolidation is a key component of the logistic strategy in the industry (Food Distributor 2000). Consolidation strategy is also often pursued with great enthusiasm (Weiskott 1998) in cases in which the products are of high value and low weight type (as in most electronics components), and when transportation costs are insignificant compared to inventory and ordering costs.

Our intent in this note is to examine the benefits of consolidation on inventory replenishment cost. Given the popularity of the consolidation strategy and the common belief that consolidation helps to reduce systemwide inventory cost resulting from risk pooling and economies of scale, we view that it is timely to scrutinize this belief based on a quantitative model. In a single-echelon system with deterministic demand in which holding and ordering costs at the retailers are not considered, it is easy to see why consolidation is optimal. In fact, in this case each warehouse acts as a single-stage EOQ system, and it is well known that the average inventory replenishment cost at each warehouse is concave in the demand assigned. Exploiting concavity

property, it is easy to see that the optimal strategy is to consolidate all demand at a single warehouse.

We show in this note that the same qualitative insight actually carries over to a two-echelon system in which both the warehouses and retailers have inventory holding and ordering costs. In a stable demand environment, where the retailer ordering costs are independent of the warehouse that services them, we show that consolidated systems are *rarely* suboptimal and *always* lead to close-to-optimal inventory replenishment costs. In particular, we prove that using two (one) properly selected warehouses, the systemwide inventory replenishment cost is in the worst case at most 2% (14.75%) more than the optimal. So the suggestion to managers facing consolidation issues with stable demand is that savings in inventory replenishment cost can often be expected, and the spotlight should thus be on the transportation costs.

We want to caution that the conclusion is reached without consideration of the impact on the operating costs in order processing, transportation, etc. We would imagine consolidation might lead to increased economies of scale in purchasing and transportation operations, but unit transportation costs could increase because the goods are now shipped over a longer distance. On another front, Teo et al. (2001), building on the work of Gallego (1998) on inventory replenishment cost approximation and bounds



Atomic Engineering of Mixed Ferrite and Core–Shell Nanoparticles

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FEATURE ARTICLE

Nanoparticulate ferrites such as manganese zinc ferrite and nickel zinc ferrite hold great promise for advanced applications in power electronics. The use of these materials in current applications requires fine control over the nanoparticle size as well as size distribution to maximize their packing density. While there are several techniques for the synthesis of ferrite nanoparticles, reverse micelle techniques provide the greatest flexibility and control over size, crystallinity, and magnetic properties. Recipes for the synthesis of manganese zinc ferrite, nickel zinc ferrite, and an enhanced ferrite are presented along with analysis of the crystalline and magnetic properties. Comparisons are made on the quality of nanoparticles produced using different surfactant systems. The importance of various reaction conditions is explored with a discussion on the corresponding effects on the magnetic properties, particle morphology, stoichiometry, crystallinity, and phase purity.

Keywords: Core–Shell Nanoparticles, Mixed Ferrites, Nickel Zinc Ferrites, Manganese Zinc Ferrites, Magnetic Properties.

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1. INTRODUCTION

In recent years the scientific literature has been replete with reports of magnetic nanoparticle synthesis, properties, and novel applications.^{1,2} This has largely been driven by the hope and in some instances the realization of surface-enhanced properties. By producing materials on the nanoscale, there exists the possibility that surface-based properties, (catalysis (or reactivity), magnetism, and electronic properties, for example) may be enhanced. In the case of magnetic nanoparticles, the disruption in crystal structure at the surface can greatly influence the magnetic properties.³ The truncation of the lattice at the surface weakens exchange interactions, in many cases reducing

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though some $4f^n-4f^n$ transition-related emissions have been observed in RE ion-doped nanocrystalline II-VI semiconductors, it was speculated that their characteristic emissions originate from RE ions adsorbed on the particle surface.¹⁰ In contrast to RE ions, the chemical properties of Mn^{2+} are very similar to those of Cd^{2+} (or Zn^{2+}), thus incorporating Mn^{2+} into II-VI semiconductor host much easier.

The Mn^{2+} ion, used in many luminescent materials, has a d^5 configuration. The Mn^{2+} ion exhibits a broad emission peak, whose position depends strongly on the host lattice due to changes in crystal field strength with host. The emission color can vary from green to deep red, corresponding to a ${}^4T_1-{}^6A_1$ transition.¹¹ Since this transition is not spin-allowed, the typical luminescent relaxation time of this emission is of the order of milliseconds.¹¹⁻¹³ Bulk ZnS:Mn has been widely used as a phosphor,¹⁴ particularly in alternating current thin film electroluminescence

(ACTFEL) devices.¹⁵⁻¹⁷ Mn^{2+} d -electron states act as efficient luminescent centers while interacting strongly with s - p electronic states of the ZnS host into which external electronic excitation is normally directed. The subsequent transfer of electron and hole pairs into the electronic level of the Mn^{2+} ion leads to the characteristic yellow emission from the Mn^{2+} ${}^4T_1-{}^6A_1$ transition.¹⁴ Possible mechanisms for excitation of the Mn^{2+} in semiconductor hosts (ZnS, CdS) have been suggested. In one mechanism a hole trapped by the Mn^{2+} ion is recombined with an electron, leading to Mn^{2+} in an excited state.^{18,19} Another suggested mechanism is recombination of a bound exciton at the Mn^{2+} site, which again promotes the Mn^{2+} to an excited state.²⁰

Although the optical properties of doped semiconductor (Mn-doped ZnS) nanocrystallines were published in 1983,²¹ it was not until the publication by Bhargava's



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