Polymer Conformational Transitions:
A Quantum Decoherence Theory Approach

D. Raković[1], M. Dugić[2] and M. Plavšić[3]

[1]Faculty of Electrical Engineering, Belgrade, Serbia and Montenegro
[2]Department of Physics, Faculty of Science, Kragujevac, Serbia and Montenegro
[3]Faculty of Technology and Metallurgy, Belgrade, Serbia and Montenegro

ABSTRACT

In this paper we describe the problem of polymer conformational transitions in the framework of the so-called quantum decoherence theory. We propose a rather qualitative scenario yet bearing generality in the context of the quantum decoherence theory. It seems that our proposal provides a promising basis for the solution-in-principle of this (semi-)classically hard problem of the polymer kinetics.

1. INTRODUCTION

Conformation is one of the most important features of polymer chains, and due to the properties dependent on conformation, very important in consideration of polymer materials, as well [1]. In parallel with standard issues of crystal- and amorphous bulk-characterization, this is especially valid for modern polymer composites, nano-structured materials and biomaterials.

But, the size of one macromolecule, with a large number of atoms and groups, able to take different configurations in space without scission of constitutional chemical bonds (what we understand as different conformations) brings problems to a different level comparing the classical approach of the conformation in organic chemistry. The large number of possible states of the system indicates statistical-mechanical approach, and strict determinism of the chemical structure leads to the quantum mechanical energy considerations.

Extreme examples for these two approaches are "random flight" model of polymer chain and *ab initio* calculation of polymer structure. The random flight model represents a macromolecule as a statistical ensemble of particles, similar to the well-known models of gas but with the effective geometrical parameters of the system, e.g. radius of gyration (R_g) equivalent to the time or ensemble averaged values for the coiled chain. Obviously, many constitutive features, important for the understanding of material properties, are lost in such a model. On the other hand, in spite of enormous increase of the power of modern computers, *ab initio* calculation is still possible only for short segments of a chain.

The first, who succeeded to incorporate within the statistical mechanical models described above some essential features of the real chain, was Flory with his excluded volume theory in 1949 [2]. The theory considers interactions of the chain links and the solvent molecules as well. It offers an elegant solution for the case when long-range chain interactions are balanced with solvent interactions (so called θ-state), and so, only short-range interactions govern the conformational geometry of the system. In essence, it is one of rear solutions for simultaneous interaction of several bodies, which is a very hard problem in physics. Later, Volkenstein, starting from the quantum mechanical approach developed the method for estimation of possible conformational states, depending on short-range interactions, called theory of rotational isomeric states [3]. In fact, the two approaches are complementary and later Flory united them in his method for the calculation of

conformational properties of polymer chains [4]. The method gave excellent agreements with experimental results obtained from light scattering and viscosity measurements for coiled chains in diluted solutions and neutron scattering in amorphous bulk materials [5]. Also scaling law from the excluded volume theory, e.g. scaling of R_g with a degree of polymerization N, has been checked by many authors and elaborated in some new mathematically extended theories, but all obtained results are practically the same as the result Flory obtained in his theory [6]. Still, there are several silent aspects in such an approach to chain conformation that should be reconsidered. The first is dynamics of the conformation transitions. Second, but following from the first, is the influence of conformational organization hierarchy on such transitions. The third is the extension of such models to biopolymers, in particular to native state of proteins. In our opinion, all three aspects are connected to quantum decoherence and transitions from quantum to classical.

1.1 Conformational transitions and the chain-folding problem

The method for the calculation of conformational dependent chain properties, considered above, describes conformational states of the system based on possible rotational states of chain bonds. It does not describe transitions between possible states of the system, i.e. transitions from one conformation to another. The first is a thermodynamic and the second is a kinetic aspect of the problem. The conformation change of long flexible chain, by random rotations around chain bonds due to thermal vibrations under the influence of the environment, has been considered understandable by itself, and included as a silent aspect in many analyses. But, literally understood it can lead to different artifacts.

This has been illustrated by Levinthal, who considered the probability of folding a protein molecule from coiled to its native conformation [7]. Assuming $2n$ torsional angles of an n-residue protein, each having three stabile rotational states, this yields $3^{2n} \approx 10^n$ possible conformations for the chain (even with rather gross underestimating). If a protein can explore new conformations in a random way, at the rate that single bond can rotate, it can find approximately 10^{13} conformations per seconds, which is here an overestimating. We can then calculate the time t(s) required for a protein to explore all the conformations available to it: $t = 10^n/10^{13}$. For a rather small protein of $n = 100$ residues, one obtains $t = 10^{87}$ s, which is immensely more than the apparent age of the universe ("Levinthal paradox"). Yet, according to some experiments, proteins can fold to their native conformation in less than a few seconds [8]. It follows that conformational changes of proteins, due to thermal, solvent and other influences of the environment, does not occur in a random way (as e.g. movements of gas particles) - but fold to their native conformation in some sort of ordered set of pathways in which the approach to the native state is accompanied by a sharp increasing conformational stability - this being one of the most crucial questions in all life sciences. Such a view some authors translate to the problem of estimations of some long range-interactions responsible in a given moment for the direction of the process [9].

The most of proteins have a part of bonds twisted (by rotation around backbone bonds - for some angle) to helical conformation. Between the helices are segments of plated sheet conformations or just turns. Such conformational elements (called secondary structure of a protein) make 3D-arrangement in space called tertiary structure. For example, globular proteins by folding the elements of secondary structure together make a globular shape of the molecule. The first who pointed to such hierarchy of conformational structures was Pauling in 1951, building in that way one of the landmarks of present structural biochemistry [10]. It should be pointed here that the density of packing secondary structure elements by folding into globular proteins shape is very dense, similar to the density of organic crystals [1]; sometimes such architecture of the protein molecule is supported by (only) several chemical bonds, linking elements of the secondary structure. The native structure of proteins is determined by tertiary organization; indeed, by unfolding protein chains due to heat or chemicals, they are denatured, not recognized and rejected by the organism [11-14]. The first who determined the tertiary structure were Perutz (on

hemoglobin) and Kendrew (on mioglobin) by X-ray diffraction studies; Perutz started research on space architecture of hemoglobin already in 1937, but the work was completed no earlier than 1957 (and of course, after Pauling provided a theoretical understanding of the secondary structure) [12,13]. While first who succeeded in renaturation of proteins, in his classical experiment of folding-back a protein to native structure, was Anfinsen in 1957, and the first who gave theoretical explanation for folding, based on statistical mechanics, was Dill [1,14].

In one quite different approach, from the field of materials science, in the late 1950s Keller succeeded in preparing single crystals of polyethylene, by nucleation in dilute solutions [15]. The crystals were platen-like shaped and of the order of 10-20 nm thick. Amazingly, electron diffraction analysis showed that the polymer chains in the crystal body were essentially perpendicular to the large flat faces of the crystal. Since the chains were known to have contour lengths of about 200 nm, and the thickness of the single crystal was ten times smaller, Keller concluded that the polymer molecules in the crystals had to be folded back upon themselves. Again one faces the problem of folding of polymer chains, confirming that it is quite a fundamental issue of polymer structure.

In this paper we seek for a solution-in-principle of the long-standing problem of the polymer folding. As we saw above this problem was considered by Levinthal as (semi-)classicaly intractable. However, herewith, we address to the fundamentals of the so-called quantum decoherence theory in order to make the problem tractable, and we propose quantum scenario as the candidate for a solution of the problem at hand. Our proposals are rather qualitative yet bearing generality in the context of the decoherence theory. Therefore, the estimates for the minimum time necessary for the polymer-conformation change cannot be made definite without referring to the more elaborate physical models. Yet, our estimates are not expected to fail in their order of magnitude, therefore making our proposals a promising basis for the solution-in-principle of the (semi-)classically hard problem of the polymer-conformation change.

2. THE (SEMI-)CLASSICAL MODEL

Due to the Born-Openheimer adiabatic approximation, the molecules can be ascribed the *definite geometrical structure* [16]. This geometrical visualization is a general feature of all kinds of molecules, from small to complex macro-ones. As to the latter, the vertices of the corresponding geometrical structure are occupied by groups of atoms or by smaller molecules.

Geometrically, the shape of a molecule can be continuously changed in 3D space. However, *only* a restricted set of the possible geometrical shapes are found experimentally. Particularly, the transformations of special interest are the so-called *conformational* transformations preserving the *spatial distances and angles* between the adjacent vertices in the geometrical shape of a molecule. Different shapes mutually related by conformational transformations are referred to as *conformations*. Every conformation is determined by the relative position in space of vortices, thus representing a *physical characteristic*, K, of a molecule *as a whole*. Therefore, as to the conformation of a molecule, one actually deals with a *one-dimensional system*, $\{K\}$. The different "values" of the variable K (i.e. the different conformations k_i) can be ascribed to different values of the molecular electronic energy as presented in Fig. 1.

The local minima of the potential-energy plot $V(K)$, Fig. 1, represent the set of preferred conformations for a molecule in a given physical situation. Actually, *in a solution*, the macromolecules exhibit both existence and stability of conformations from a given set of possible shapes, which are exactly presented by the local minima of the potential energy $V(K)$.

Needless to say, the geometrical shape of a molecule is not frozen, thus giving rise to the fast oscillations of the shape around the actual conformation - e.g., k_i in Fig. 1. Therefore, the one-dimensional system K can be modeled as a one-dimensional quasiparticle with the position K and the conjugate momentum P, oscillating with some typical frequency ω_i around the bottom of the actual local minimum, say k_i of Fig. 1.
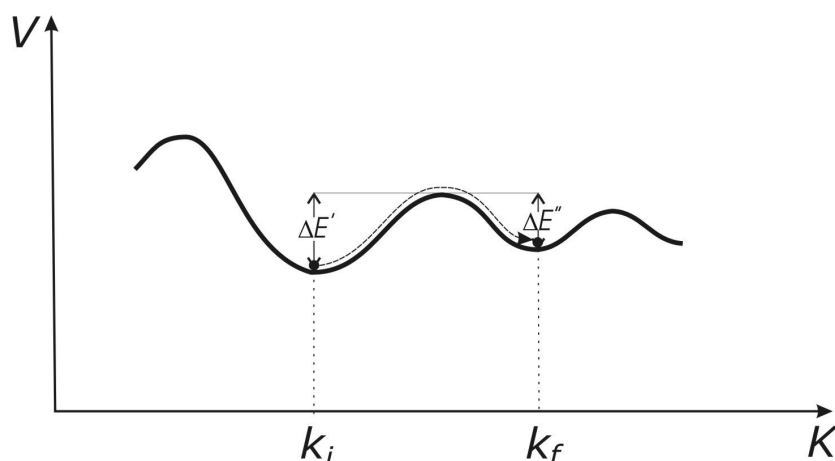
Fig. 1. The molecular electronic energy as a potential energy for the adiabatically decoupled (vibrational and) one-dimensional conformational system K. The local minima are the semi-classically stable "positions" in the K-space. However, rather fast transitions from *initial* to *final* conformations ($k_i \to k_f$, with corresponding conservation laws and selection rules fulfilled) cannot be treated (semi-)classically, but necessarily within the general framework of the quantum decoherence theory (see Sect. 3.2 for our approach).

The (semi-)classical model of Fig. 1 *encapsulates the up-to-date experimental evidence* on the conformations of macromolecules, distinguishing the stability of the preferred set of conformations of a molecule *in a solution*[1]. In a *"stationary state"* when no external action on the system is performed, the conformations are preserved due to, among else, the high-energy barrier between the adjacent local minima of Fig. 1. Physically, this means that the oscillator does not have enough energy to skip over the barrier in order to change its geometrical shape; such shape-transitions (conformation changes) can be formally presented by $k_i \to k_f$ (the indices i and f standing for *initial* and *final* conformations, respectively).

However, some external actions on the solution (e.g., thermal, compositional, optical, etc.) result in a change of conformation of a molecule that can be experimentally observed/verified. Thus, effectively, the external action gives rise to the transitions of the type $k_i \to k_f$ for a molecule in a solution, in general giving rise to different kinds of transformations for different molecules. These transformations can take different time intervals to affect themselves, which can be estimated from the experimental data. First, there are the *spectroscopic* data suggesting the orders of 10^{-9} s for the conformation changes [17]. Second, the duration of typical experiments in this regard (protein renaturing [8]) is of the order of 1 s. Needless to say, the time interval (10^{-9} s, 10^0 s) is in *sharp contradistinction* with the existing *(semi-)classical* predictions. And this is the very heart of the polymer conformation transitions (PCT).

Actually, from a (semi-)classical point of view, the change of conformations *requires* a sequence of local *non-commuting* successive transformations (rotations), whose number is so *large* that the total time for exploring all the conformations available becomes *unreasonably long* [7]. Needless to say, every single elementary transformation (local rotation) is a continuous map in 3D space. Therefore, the whole transformation (net transformation of the shape of a molecule), $k_i \to k_f$, can be ascribed to the *unique trajectory* in K-space connecting the initial (k_i) and the

---

[1] *In a solution*, a molecule can*not* take arbitrary geometrical shape. Only the conformations from a *preferred set* are available. Actually, it seems that the *local interactions* (between the macromolecule and the solvent molecules) give rise to both, the choice of the preferred set of conformations and the stability of conformations; as to the latter, in a solution, when no external action on the system is performed, a macromolecule *maintains* its geometrical shape exactly as presented by the model of Fig. 1.

final (k_f) conformation. Given that the net transformation can be performed *only in a succession of* n_e *elementary transformations* (local rotations), the problem arises when, even for arbitrarily small time interval, τ_e, of the elementary operations, the time necessary for the net transformation, $\tau \equiv n_e \cdot \tau_e$, is unreasonably long time interval.

3. QUANTUM MECHANICAL MODEL

Our approach to *PCT* bears *complete generality*. We refer neither to the specific polymers (or solutions) nor to the specific conformations. In this section we give the basics of our approach and prepare for the details of the scenario, which might be the basis for the final solution of *PCT*.

3.1 Quantum decoherence effect: the fundamentals

Fulfilling the conditions of existence and of stability of conformations is our first objective. Fortunately, a straightforward application of the so-called decoherence theory [18] suffices in this respect.

The general physical situation may be presented as follows. A quantum system S is in unavoidable interaction with its environment E. The composite system $S+E$ is subject to the Schrodinger law. However, then, neither S nor E is subject to the Schrodinger law. Such systems are referred to as the *open quantum systems*. The task is to calculate the (open) system's (S's) state - the so-called "reduced statistical operator" - denoted by $\hat{\rho}_S$. The (sub)system's state is defined as:

$$\hat{\rho}_S(t) = tr_E \left(\hat{U}(t) \hat{\rho}_{S+E}(t=0) \hat{U}^*(t) \right) \tag{1}$$

where $\hat{U}(t)$ is the unitary operator of evolution in time, $\hat{\rho}_{S+E}(t=0)$ is the initial state of $S+E$ system, while "tr_E" refers to the integrating over the environmental degrees of freedom.

Under the set of special conditions [19], one can observe the *occurrence of the decoherence effect* defined loosely as:

(i)   in the representation of a special orthonormalized basis, $\left\{ |i\rangle_S \right\}$ of the (Hilbert) state space of S - the so-called "pointer basis" - one obtains *disappearance of the off-diagonal elements* of $\hat{\rho}_S$:

$$\lim_{t\to\infty} \rho_{Smm'}(t) = 0, m \neq m' \tag{2}$$

(ii)   with the requirement of *stability ("robustness")* of the elements of the pointer basis:

$$\hat{H}_{int} |i\rangle_S |\varphi\rangle_E = |i\rangle_S |\varphi_i\rangle_E \tag{3}$$

or equivalently

$$\hat{U}(t) |i\rangle_S |\varphi\rangle_E = |i\rangle_S |\varphi_i(t)\rangle_E . \tag{4}$$

Then, effectively, there appear the *environment-induced superselection rules (decoherence)*, which *forbid the coherent superpositions of certain states of the system S*. In other words, decoherence *establishes existence and robustness* of a preferred set of states - e.g. of the "pointer basis" - of an open system.

If the initial state of S is a coherent superposition, $|\psi\rangle = \sum_i c_i |i\rangle_S$, then the decoherence process can be presented as:

$$|\psi\rangle = \sum_i c_i |i\rangle_S \xrightarrow{\tau_D} \hat{\rho}_S = \sum_i |c_i|^2 |i\rangle_S {}_S\langle i| \tag{5}$$

where τ_D, the *decoherence time,* is the order of magnitude of the unfolding the decoherence process. Eq. 5 exhibits the loss of the initial coherence - which justifies the term *de*coherence [18].

Now, as to our task, it suffices properly to model the interaction Hamiltonian, $\hat{H}_{int}$, in order to deduce (i) and (ii), i.e. Eq. 5 for the composite system "conformation + environment $(K+E)$". Needless to say, with this, we would deduce the phenomenologically observed existence and stability of a preferred set of conformations.

Without employing any details, we emphasize that virtually independent on the model of the system E, the following simplest separable interaction Hamiltonian fulfills our requirements (being necessary condition for decoherence effect) [19]:[2]

$$\hat{H}_{int} = C\hat{K}_K \otimes \hat{D}_E , \tag{6}$$

where C stands for the coupling constant (determining the strength of interaction), $\hat{K}_K = \sum_i k_i |k_i\rangle_K \,_K\langle k_i|$ is the conformation observable of the quantum system K, and $\hat{D}_E$ is arbitrary observable of the environment E.

3.2 General quantum-mechanical scenario for polymer conformational transitions

By applying the fundamentals of the quantum decoherence theory, we are able to reproduce the basics of the classical model for the macromolecule conformations for the stationary situation when no external action on the system is performed. However, our problem refers to the situations when the external action on the system results in the *change of the conformations*, which is the subject of this subsection.

In this subsection, we outline the *sufficiently general* quantum-mechanical model that may account for the effect of change of conformation in *short time intervals* - in obvious contradistinction with the results of the (semi-)classical physics analysis. The generality of our considerations allows applicability of the model for different yet *realistic* physical situations, thus eventually presenting a basis for the final solution of the problem at hand.

The condition (ii) of Sect. 3.1 exhibits a special characteristic of the decoherence process: decoherence tends to freeze dynamics of an open system, once the system is in a "preferred" state. Therefore, our task here reads: to model the external influence on the system $K+E$ so as to both first to break and later to re-establish the effect of the decoherence due to the interaction, Eq. 6.

We introduce the following, *physically and phenomenologically plausible* assumptions: (i) the external influence is much stronger than the interaction Eq. 6, and (ii) *after* the external action, the composite system relaxes to equilibrium (a stationary state) determined by the model Eq. 6.

Before the external action, K's stationary state reads:

$$\hat{\rho}_K = \sum_i |c_i|^2 |k_i\rangle_K \,_K\langle k_i| . \tag{7}$$

The strong external action on the $K+E$ system of the duration T_{ext} (providing, for instance, the external energy $\Delta E'$ to skip over barrier in order to change its conformations from k_i to k_f, in two-conformational example of Fig. 1) gives rise to the following nonstationary state transformation for the system K:

$$\hat{\rho}_K \rightarrow \hat{\rho}_K ' , \tag{8}$$

---

[2] The interaction Hamiltonian (6) is the *simplest possible form* of the class of the so-called *separable interactions* [19], *equivalent* in its spectral form to *more general form* $\hat{H}_{int} = \sum_i C_i \hat{A}_{Ki} \otimes \hat{B}_{Ei}$, as long as $\left[\hat{A}_{K_i}, \hat{A}_{K_j} \right] = 0$, $\left[\hat{B}_{E_i}, \hat{B}_{E_j} \right] = 0$, for every pair of indices i,j, and if the conformations $\left\{ |k_i\rangle_K \right\}$ represent a common eigenbasis for the set $\left\{ \hat{A}_{Ki} \right\}$.

so that, *in general*:

$$[\widehat{\rho}_K, \widehat{\rho}_K{}'] \neq 0 . \tag{9}$$

After the external action, the composite system *K+E'* is subject to the nonstationary *relaxation process* of the duration T_{rel} (taking-off, for instance, the excess external energy $\Delta E''$ to fulfill energy conservation law in two-conformational transition $k_i \to k_f$ of Fig. 1) which in general gives rise to another state change of *K*:

$$\widehat{\rho}_K{}' \to \widehat{\rho}_K{}''. \tag{10}$$

The relaxation process *re-establishes* the stationary state defined by Eq. (6), which - *and this is the point strongly to be emphasized* – guarantees the existence and stability of conformations. That is, the final state of the system *K* reads:

$$\widehat{\rho}_K{}''' = \sum_i w_i \, |k_i\rangle_K \, {}_K\langle k_i|. \tag{11}$$

The occurrence of the final state of the form Eq. 11 can be easily proved [19].

Now, the point is in the difference of the initial $\widehat{\rho}_K$ and the final $\widehat{\rho}_K{}'''$. Both states refer to the conformations $|k_i\rangle_K$ guaranteeing their existence and stability. However, the relative number (concentration) of different conformations - i.e. the "statistical weights", w_i - are likely to be different, $w_i \neq |c_i|^2$. *In effect*, there has occurred a change of conformation, at least for a sample of molecules in a solution - *which is exactly the effect we search for*.

The total duration of the effect reads:

$$T = T_{ext} + T_{rel} + \tau_D , \tag{12}$$

where τ_D refers to the duration of decoherence effect: $\widehat{\rho}_K{}'' \to \widehat{\rho}_K{}'''$. Since it is expectable [18]:

$$T_{ext} + T_{rel} \gg \tau_D \tag{13}$$

the *duration of the conformation change in our model is of the order of* $T_{ext} + T_{rel}$ - in obvious contradistinction with the estimates based on the (semi-)classical analysis.

4. DISCUSSION

The core of the (semi-)classically addressed problem is the unreasonably long time necessary for the change of conformations of a polymer in a solution. Therefore, every sound physical model overcoming this problem deserves consideration as a potential basis of the final solution of the problem. To this end, the scenario of Sect. 3.2 obeys this criterion. The new element in this regard is that we employ the *fully* quantum-mechanical models for the *open system* of interest, *K*, in unavoidable interaction with its environment, *E*. More precisely: we employ the foundations of the decoherence theory for both, existence and stability of the conformations, *and* for the processes of the change of conformations in the nonstationary state of the composite system $K + E$.

Without referring to a concrete model of the composite system $K + E$ (i.e. $K + E'$), one cannot make sufficiently general estimates of the characteristic time intervals for different processes analyzed in Sect. 3.2. Fortunately enough, from the general decoherence theory, it is expectable (plausible to suppose) that the decoherence time τ_D is by many orders of magnitude the shortest time interval for the scenarios (models) considered. Therefore, it is plausible to suppose that *generally*, the duration of the change of conformations is of the order of $T_{ext} + T_{rel}$, as emphasized in Sect. 3.2. This observation, in our opinion, encourages further investigations of the model *in order to make the connection to the concrete physicochemical situations* that are in principle

experimentally testable. Needless to say, only such kind of the experimental tests might represent the decisive step in resolving the problem of interest.

It should be also pointed out, that the proposed quantum-decoherence model might be generalized on any quantum system and its quasiparticle's excitations, as the analogous energy-state plot, $E(\phi)$ (cf. Fig. 1) is the general quantum-informational characteristics of any quantum-system in Feynman's representation [20]. Therefore, this poses a new light on the existence and stability of any kind of the condensed-state more or less delocalized quasiparticles (electrons, phonons, conformones, etc.) and their rather fast excitations (with characteristic times and frequencies, as a consequence, only slightly dependent on dimensions of the condensed-state system [17]) in the proposed framework of the general quantum decoherence theory - implying a fuzzy borderline between quantum coherent (nonstationary) and semi-classical decoherent (stationary) manifestations of any macroscopic condensed-state system (see for instance [21]).

5. CONCLUSION

Employing the fundamentals of the decoherence theory, we are able to reproduce both, existence and stability of the polymers conformations, *and* the short time scales for the quantum-mechanical processes resulting effectively in conformational transitions. The proposed model is certainly not exhaustive yet providing us possibility to *overcome the main obstacle* in resolving the problem of interest - the problem of (semi-)classically unreasonably long time necessary for the change of conformations of the polymers in a solution. Also, it is general enough to provide wider framework for both existence/stability and fast excitations of any kind of the condensed-state delocalized quasiparticles.

REFERENCES
[1] M. Plavšić, Polymer Materials Science and Engineering, Naučna knjiga, Belgrade (1996), in Serbian.
[2] P. Flory, J. Chem, Phys., **17**, 303 (1949).
[3] M. V. Volkenstein, Configurational Statistics of Polymer Chains, Interscience-Wiley, New York (1963), transl. from Russian ed. (1959).
[4] P. J. Flory, Principles of Polymer Chemistry, Cornell Univ. Press, Ithaca (1953); P. Flory, Statistics of Chain Molecules, Interscience-Wiley, New York (1969).
[5] J. P. Cotton, D. Deches, H. Benoit, B. Fornoux, C. Picot, G. Jaunink, R. Ober, J. de Cloiseaux, Macromolecules, **7,** 863 (1974).
[6] M. Fixman, J. Chem Phys., **45**, 785 (1966), and references therein.
[7] C. Levinthal, J. Chem. Phys., **65**, 44 (1968).
[8] C. B. Anfinsen, Science, **181**, 223 (1973), and references therein.
[9] P-G. De Gennes, Scalling Concepts in Polymer Physics, Cornell Univ. Press, Ithaca (1979).
[10] L. Pauling, B. R. Corey, H. R. Branson, Proc. Natl. Acad. Sci. USA, **37,** 205 (1951).
[11] D. Voet, J. G. Voet, Biochemistry, Wiley, New York (1995).
[12] M. F. Perutz, Nature, **228**, 726 (1970).
[13] J. C. Kendrew, Science, **139**, 1259 (1963).
[14] K. A. Dill, Biochemistry, **24**, 1500 (1985).
[15] A. Keller, Phil. Mag., **2**, 1171 (1957).
[16] L. A. Gribov, W. J. Orville-Thomas, Theory and Method of Calculation of Molecular Spectra, Wiley, New York (1988).
[17] D. Raković, Physical Bases and Characteristics of Electrotechnical Materials, Faculty of Electrical Engineering, Belgrade (1995), in Serbian.
[18] D. Giulini, E. Joos, C. Kiefer, J. Kupsch, I. –O. Stamatescu, H. D. Zeh, Decoherence and the Appearance of a Classical World in Quantum Theory, Springer, Berlin (1996).
[19] M. Dugić, Phys. Scripta, **56**, 560 (1997).
[20] M. Peruš, Neural Network World, **10**, 1001 (2000).
[21] C. A. Chatzidimitriou-Dreismann, T. Abdul-Redah, and R. M. F. Streffer, J. Chem. Phys., **116,** 1511 (2002).

Progress in Advanced Materials and Processes

Polymer Conformational Transitions: A Quantum Decoherence Theory Approach