Preface

As a volume in the *Shock Wave Science and Technology Reference Library*, this book is primarily concerned with the fundamental theory of detonation physics in gaseous and condensed-phase reactive media.

A detonation is a chemical reaction transport process accompanied by high-speed energy release. It comprises a shock wave standing upstream of the chemical reaction, where both propagate as a tightly coupled complex with supersonic velocity (2–10 km/s). After the passage of the detonation wave, the reactive medium is transformed into high temperature and pressure gaseous products, thereby providing enormous thermodynamic work potential for commercial and military applications. The detonation process involves complex interactions between reactive chemical dynamics and fluid dynamics, accompanied by intricate effects of heat, light, electricity and magnetism. These characteristics make detonation dynamics an important field of applied physics, spanning numerous theoretical and applied research topics. Outstanding summaries of the fundamental physics and theory of detonation can be found in a number of classic books (e.g., Zeldovich, Ya.B., Kompaneets, A.S.: Theory of Detonation, Academic Press, New York, 1960; Soloukhin, R.J.: Shock Waves and Detonations in Gases, Mono Book Corp., Baltimore, 1966; Fickett, W., Davis, W.C.: Detonation, University of California Press, Berkeley, 1979). A recent book "The Detonation Phenomenon" by J.H.S. Lee (Cambridge University Press, Cambridge, 2008) offers a very informative reading on the up-to-date phenomenology of gaseous detonation physics. The current book, however, tries to address the recent developments in the theoretical foundation of detonation physics, in both gaseous and condensed-phase energetic materials. The book contains seven chapters which were written by a number of subject experts. The chapters are thematically interrelated in a systematic descriptive approach, where each chapter is self-contained. It offers a timely reference in theoretical detonation physics for graduate students as well as professional scientists and engineers.

The first chapter, by Sorin Bastea and Laurence E. Fried, describes the equilibrium Chapman–Jouguet (CJ) detonation theory. The CJ theory

simplifies the detonation wave to a strong discontinuity after which the flow is sonic with chemical reaction complete at an equilibrium detonation products state. With a brief introduction to the classic CJ theory, the chapter focuses on modern challenging topics of equilibrium detonation with emphasis on condensed-phase energetic materials. These subjects include the equations of state and high pressure chemistry and physics of detonation products such as dissociation, ionization and phase separation. Conditions and limitations are discussed for applying the theory to practical explosives with finite size and heterogeneity. This chapter offers a solid foundation for the application of modern equilibrium detonation theory to increase predictability in computing macroscopic average detonation states for a wide variety of both existing and novel energetic materials.

The simplicity of the CJ theory prevents one from gaining insights into the variety of detonation wave structures responsible for detonation propagation, initiation and failure. The second chapter, by Andrew Higgins, introduces the Zeldovich, von Neumann and Döring (ZND) model that emerged in the 1940s to offer a steady planar reaction zone structure of detonation. The chapter then provides a state-of-the-art description of generalized, steady, quasi-one-dimensional detonation theory, in which the rate of energy loss competes with the rate of exothermic chemical energy release within the reaction zone, thus resulting in the flow passing a sonic point at a chemically non-equilibrated state. The energy loss inherent in the materials or its boundaries has been systematically depicted in the chapter through endothermic chemical reaction, friction, heat loss and flow divergence. The common characteristics and differing varieties of steady detonation zone structures are discussed under various energy loss mechanisms through the coupling of the chemical reaction and fluid dynamics. This chapter provides a one-dimensional average framework upon which the detonation instability and multidimensional structures are built. The generalized ZND detonation theory also offers a foundation to predict detonation performance of nonideal energetic materials.

Numerous experiments since 1959 have demonstrated that the dynamic trajectory of a detonation wave front generally manifests itself as an unsteady, non-planar cellular structure in both homogeneous and a number of heterogeneous materials. The steady one-dimensional ZND detonation structure is theoretically unstable and will be transformed into an ordered unsteady oscillating structure under given conditions. The third chapter, by Hoi Dick Ng and Fan Zhang, describes the fundamental theory of detonation instability and its recent development. The kernel of unstable detonation theory lies within a nonlinear dynamics consideration, in which the oscillating instability modes generally transit through a period bifurcation or trifurcation sequence to chaos. After an introduction to classic linear stability analysis, the chapter presents in detail this latest nonlinear detonation instability theory in one-dimensional space. This theory helps to reveal the hidden nature of the reactive fluid dynamics equations, where the coupled chemistry dominates the control parameters for instability transition. The effect of coupled chemistry

on the detonation instability is further addressed through different reaction kinetic models. Recent two-dimensional numerical simulations also confirm the instability hierarchy of detonation cellular structure in the same bifurcation sequence, with additional multidimensional effects including transverse waves and turbulent mixing to help us move towards a quantitative description of cellular detonation instability. Finally, nonideal detonation instability is analyzed, where the dissipation resulting from energy loss sources create an additional class of stability control parameters that lead to detonation velocity reduction and instability.

The fourth chapter, by Anatoly Vasil'ev, provides a fundamental description of dynamic parameters of cellular detonation in gaseous mixtures with an emphasis on the theoretical analysis, mostly from the author's own distinguished studies, accompanied with numerous experimental data. The dynamic parameters described in this chapter include detonation cell size, critical energy for direct initiation of detonation and critical opening size for detonation diffraction re-initiation. These subjects are followed by an introduction to advanced schemes for detonation initiation and critical geometry scales of limiting detonation waves. The theoretical models capture the essential detonation phenomenon of transverse wave collisions as local explosions to form detonation cells; their agreement with a large quantity of experimental data demonstrates an adequate functional relation between critical initiation energy and cell size. This chapter lays out a theoretical foundation for the calculation of dynamic parameters of the regular cellular detonation, as well as the irregular cellular detonation with a dominant mean cell size.

The fifth chapter, by Daniel Desbordes and Henri-Noël Presles, offers an informative review of recent advances in the area of gaseous detonation cellular structure. The detonation cellular structure has been characterized by a main cell size that is deduced from a cell size spectrum and may contain substructures, depending on the degree of detonation instability. The authors of this chapter, along with their coworkers, have newly discovered a two-cell structure where a large cellular structure is superimposed on that of smaller cells, thus opening an avenue which extends existing detonation physics and theory. This chapter begins with an overview of the experimental observation of various detonation wave structures including the latest finding of two-cell structure. It then presents a detonation energy release theory, in which the traditional cellular structure dominated by one main cell size, is replicated by one-step chemical heat release with one peak of thermicity, while the two-cell detonation structure is a result of two-step heat release with two maxima in thermicity within the ZND detonation reaction zone. Between the two models, there is a transition regime where the two-step heat release only exhibits one peak in thermicity. This theory is applied in direct numerical simulations to predict various cellular detonation structures in different mixtures, and in an attempt to explain disputed critical problems including detonation diffraction re-initiation and the limiting detonation in tubes. The multi-cell detonation wave might display a more comprehensive structure for mixtures of multiple

fuels with different chemical kinetic length scales as the reacting flow moves towards the sonic point. Hence, the theory invoked in this chapter, if valid, might be extended to a multi-scale heat release law with multiple maxima in thermicity to predict multi-cell detonation structure. While the detonation propagation, transmission and instabilities have been associated with the role and type of transverse waves, detonation chemistry is no doubt dominant in controlling the dynamics of cell structure.

The description in Chaps. 2–5 primarily uses gas as a prototypical material, because the inherent low density permits sufficient observation resolution. It is expected that the range of applicability of the main principles described in these chapters would extend to detonation in generic homogeneous energetic materials including liquid and solid, as well as in a number of heterogeneous materials (see Heterogeneous Detonation, Volume 4 of *Shock Wave Science and Technology Reference Library*).

Due to high material density and detonation pressure of the order of tens of gigapascals, the condensed-phase detonation structure has been a subject of debate between nonequilibrium thermal initiation behind the shock front and nonequilibrium mechanical initiation within the shock front. Experimental support to answer these questions must be derived under extreme conditions of pressure from observations within the shock front, thereby requiring measurement resolution on the tens of femtosecond time scale. The sixth chapter by Craig M. Tarver presents an overview on the development and challenge towards a condensed matter detonation theory. The author proposes a nonequilibrium ZND model based on the timescale analysis of various nonequilibrium processes. While much more research will be required to fully understand the nonequilibrium processes coupled with the high pressure chemistry to establish a condensed matter detonation theory, the chapter also offers a simple phenomenological reaction model of ignition and growth, and its use in practical detonation modeling in comparison with a number of experiments.

The last chapter, by John B. Bdzil and D. Scott Stewart, systematically describes the fundamentals of detonation shock dynamics (DSD) as a technique to efficiently compute engineering-scale effects of condensed-phase detonation. A detonation wave front for condensed-phase energetic materials, from a macroscopic average view point, generally experiences curvature in the vicinity of an inert lateral boundary. The detonation velocity is influenced by this front curvature and can experience a strong deficit due to divergent flow. In the DSD theory, the relationship between the normal detonation velocity and the front curvature therefore plays a key role. The authors of this chapter have laid the main foundation for the rigorous development of modern DSD theory. They extended Whitham's geometrical inert shock dynamics to a detonation shock evolution through an asymptotic theory applied to the quasi-one-dimensional ZND detonation model. This chapter offers a rigorous derivation and description of the theory in a gradual and logical fashion. It clearly demonstrates the superiority of this theory over the classic Huygens formulation where the detonation velocity is assumed to be constant. It also

shows great potential for high simulation efficiency in engineering-scale explosive applications when the DSD theory is coupled with the numerical solution of the flow field behind the detonation. This precludes the necessity to apply expensive, multidimensional simulations with sufficient resolution to capture the correct solution within the 10^{-5} m or less thickness of the detonation reaction zone.

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