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A microscopic model for the propagation of detonations in solids

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Abstract. We present a simple one-dimensional microscopic model for the propagation of a detonation which is specially adapted to solids. It couples a non-linear equation for the dynamics of the crystal lattice to an equation describing the molecular dissociations. Analytical calculations in the continuum limit and numerical solutions of the discrete model show that it yields the essential features of a detonation wave. Moreover, the model exhibits the existence of two detonation regimes, in agreement with recent molecular dynamics simulations.

1. Introduction

Fundamental studies of detonations are interesting for two reasons: first, because extreme conditions prevail in a detonation wave, it can be used to probe interatomic forces in regions which are hardly accessible by any other means; second, the detonation couples a shock wave and a chemical reaction, i.e. it involves mechano-chemistry about which very little is known. However, while the understanding of detonations in gases or fluids has made significant progress in the last decade, the *microscopic* structure of detonations in solids is far from being understood [1]. As direct observations are difficult due to the space and time scales involved, molecular dynamics simulations have been used to determine the microscopic structure of detonation waves in crystals [2, 3, 5–8]. However, these simulations are comparable to an experiment in the sense that we can only use them to observe the properties of a given system under different conditions. Although we have a much better control over the system than in a real experiment, and although we can vary model parameters to analyse the mechanisms of the detonation, the obstacle to a fundamental understanding is that we are still dealing with a very complicated system. In a typical simulation, an atom is subjected to tens of interactions from its neighbours. This is why simple one-dimensional models restricted to the basic mechanisms of the detonation, namely the propagation of a shock coupled to a chemical reaction, are useful. Many such models of detonations have already been proposed and they have reached a level where they describe not only the propagating front but also its instabilities, oscillations, etc [9]. However they treat the case of gases or fluids where hydrodynamics and reaction diffusion equations provide a good description. The case of a solid is fundamentally different both from the point of view of the chemistry and of the shock wave, because, in the vicinity of the detonation front, there is no atomic diffusion and it is not possible to represent the motions of the lattice by a heat diffusion equation which is of parabolic type. Instead an hyperbolic equation describing wave propagation is required. Moreover, as the shock front

is very narrow on the molecular scale [8], a model which preserves the discreteness of the lattice is important.

We present here a simple model for the propagation of a detonation which takes into account the specificity of the solid state. The motivation to establish such a model is that, in its design, we make assumptions on the mechanisms which dominate the propagation of the detonation, and then, if the model can reproduce satisfactorily the molecular dynamics and experimental results, the validity of these assumptions is confirmed, and we have gained some understanding of the detonation process. The aim of our approach is not to propose a quantitative analysis of the vast number of experimental data which are available on solid detonations, but to discuss a possible path toward a fundamental understanding of the process. This is why the model has been kept as simple as possible, and, in particular, one dimensional.

2. Design of the one-dimensional model

The essence of the detonation process is the coupled propagation of a shock wave and a chemical reaction which assist each other through their coupling. Therefore the model must include these two aspects. We have chosen for each of them a description which is as simple as possible, but contains the fundamental physical properties. We consider a lattice made of molecules which can undergo an exothermal chemical reaction. We start from well known models for the propagation of a shock wave and a chemical reaction, which are then modified to take into account the specificity of the detonation in a solid, and to introduce the coupling between the shock and the reaction.

2.1. Model for the shock wave

We restrict our attention to plane waves in which the wave plane is orthogonal to the direction of the propagation of the detonation. This assumption reduces the lattice model to a one-dimensional problem, so that the lattice can be viewed as a simple chain of atoms of mass m . Due to the very large lattice distortions which are observed in a detonation wave where the average volume of unit cell particles can be reduced to less than 60% of its equilibrium value, the interaction potential between the atoms cannot ignore the non-linearity. We have considered the first non-linear term in the expansion of the potential around its minimum by introducing cubic anharmonicity in the potential

$$V(r) = \frac{1}{2}Gr^2 + \frac{1}{3}Ar^3 \quad (\text{with } A < 0) \quad (1)$$

where r is the relative distance of the atoms which interact. If we denote by $R_i(t)$ the displacement of atom i with respect to its equilibrium position, the Hamiltonian of the lattice is

$$H = \sum_i \frac{1}{2} \left(\frac{dR_i}{dt} \right)^2 + V(R_{i+1} - R_i) \quad (2)$$

so that the equation of motion of atom i is

$$m \frac{d^2 R_i}{dt^2} = G(R_{i+1} - 2R_i + R_{i-1}) + A [(R_{i+1} - R_i)^2 - (R_i - R_{i-1})^2]. \quad (3)$$

Although no restriction is imposed on the amplitude of the displacements which can be very large and thus strongly excite the non-linearities, such a model assumes that the sequence of the atoms in the lattice (determined by index i) is not destroyed. Therefore the

model does not describe the gas phase which is well behind the shock on the atomic scale. We are interested here in modelling the early stage of the chemical reactions which occur in the immediate vicinity or even within the shock front [3, 4], i.e. in a region where the lattice structure, although it is extremely distorted, is not completely destroyed.

It is interesting to introduce the relative stretching of a bond as $U_i = (R_i - R_{i-1})/a$, where a is the equilibrium distance between the atoms because, in some limits, it leads to equations having analytical solutions. The equation of motion of the lattice can be written as

$$m \frac{d^2 U_i}{dt^2} = G(U_{i+1} - 2U_i + U_{i-1}) + A [U_{i+1}^2 - 2U_i^2 + U_{i-1}^2]. \quad (4)$$

Such a discrete model has supersonic soliton-like solutions which provide an approximate description of the shock wave [10]. Since the numerical solutions show that, in solid phase detonations, the width of the shock front can be as narrow as a few lattice spacings, the discrete description provided by equation (4) is essential to represent accurately the shock, but no analytical solution of this coupled set of non-linear differential equations is known. An approximate expression, which is qualitatively correct, can be obtained in the continuum limit where $U_i(t) \rightarrow u(x, t)$. Keeping only the leading non-linear and dispersive terms, equation (4) reduces to the well known Boussinesq equation

$$u_{tt} - c_0^2 u_{xx} - p(u^2)_{xx} - hu_{xxx} = 0 \quad (5)$$

where the subscripts denote partial derivatives and $c_0^2 = Ga^2/m$, $p = Aa^3/m$, and $h = Ga^4/12m$. This equation has the soliton solution

$$u(x, t) = -\frac{A_0}{L} \operatorname{sech}^2[(x - vt)/L] \quad (6)$$

with amplitude $A_0 = 3[h(v^2 - c_0^2)]^{1/2}/|p|$ and width $L = 2[h/(v^2 - c_0^2)]^{1/2}$. The continuum limit expression $r(x, t)$ of the atomic displacements $R_i(t)$ is obtained from

$$\begin{aligned} \frac{dr(x, t)}{dx} &= u(x, t) \\ \lim_{x \rightarrow +\infty} r(x, t) &= 0 \text{ (no displacement ahead of the shock)} \\ \lim_{x \rightarrow \pm\infty} r_x(x, t) &= 0 \text{ (steady state far from the shock)} \end{aligned}$$

which give

$$r(x, t) = A_0 \left(1 - \tanh \frac{x - vt}{L} \right). \quad (7)$$

This kink-shaped solution is in qualitative agreement with our numerical calculations. In particular, molecular dynamics shows that faster shocks are narrower in agreement with the expression for L .

To complete the lattice model for the detonation wave, one must however add two physical phenomena to equation (3). The first one is the coupling with the chemical reaction, which will be discussed below, and the second one is the coupling with other degrees of freedom in the lattice, in particular with transverse motions. This coupling is responsible for an energy transfer to modes which are not explicitly included in the model, causing a damping of the shock wave. In our approach, this effect is modelled by a phenomenological damping term $-\gamma dR_i/dt$ added to the RHS of equation (3).

2.2. Model for the chemical reaction

The chemical model must describe the kinetics of the dissociation of the molecules. As for the lattice model it is derived from a well known model for the propagation of a chemical reaction which will be suitably modified to take into account the peculiarity of the solid phase detonation and introduce the coupling with the shock wave. We restrict our attention to plane waves, so that we consider again a one-dimensional model. We denote by $\Phi_i(t)$ (or $\phi(x, t)$ in the continuum limit) the portion of the molecules which are dissociated in the i th column of the lattice (or at position x). Ahead of the reaction front $\Phi_i = 0$ while far behind the front, $\Phi_i = 1$.

As a basis for the chemical model we have chosen the model of Schlögl and Berry [11]. This is a model for chemical reactions in a fluid phase, where the evolution of ϕ is determined for one part by the rate function which describes the kinetics of the chemical reactions involved, and for a second part by the diffusion of the species according to the equation

$$\frac{\partial \phi}{\partial t} = K\phi(\eta - \phi)(\phi - 1) + d \frac{\partial^2 \phi}{\partial x^2} \quad (8)$$

where K and η are two constants which are determined by the kinetic constants of the chemical reactions, and d is the diffusion coefficient of the species. For $\eta \leq 0.5$, the model has a solution which describes the propagation of a reaction front of width L_R at constant speed v_R according to the equation

$$\begin{aligned} \phi(x, t) &= \left\{ 1 + \exp \left[\sqrt{\frac{K}{2d}} \left(x - \sqrt{\frac{Kd}{2}} (1 - 2\eta)t \right) \right] \right\}^{-1} \\ &= \left\{ 1 + \exp [(x - v_R t)/L_R] \right\}^{-1} \end{aligned} \quad (9)$$

with $v_R = \sqrt{(Kd/2)}(1 - 2\eta)$, and $L_R = \sqrt{(2d/K)}$. This solution has a kink shape, with $\phi \rightarrow 0$ for $x \rightarrow +\infty$, corresponding to the unreacted region ahead of the shock, and $\phi \rightarrow 1$ for $x \rightarrow -\infty$, corresponding to the fully reacted region behind it. This model can describe, for instance, the propagation of a combustion in a fluid and is consequently well adapted as a starting point to describe the chemical reaction in the detonation wave.

2.3. Model for the detonation wave

In order to derive a model for the propagation of a detonation, we need to modify and complete the models described above for a shock wave and a reaction wave propagating independently of each other, in order to introduce the coupling between the two processes which is the essence of the detonation.

The local effect of the chemical reaction to sustain the shock wave takes place in the region where the energy is released, i.e. within the reaction front. Ahead of the front the molecules have not yet released their energy, while behind it the energy release is over. Consequently the effect of the reaction on the dynamics of the atoms can be represented by adding to equation (3) a term $-\alpha(\Phi_i - \Phi_{i-1})/a$ which is proportional to the slope of the reaction front around site i . The negative sign is necessary so that the reaction front, which has a negative slope ($d\phi/dx < 0$), sustains the shock by giving a positive acceleration to the atoms, and the constant α determines the strength of the coupling between the reaction and the shock, i.e. the efficiency of the reaction to sustain the shock.

In order to describe a solid phase detonation, equation (8) for the chemical reaction must be modified because, in the solid, there is no diffusion of the species. The term

$\partial^2\phi/\partial x^2$ must be removed from the equation. The role of this term was to introduce a coupling between different spatial points in the system. In the case of a detonation, the spatial coupling is due to the propagation of the shock in the lattice, which is the mechanism by which 'information' is transmitted from one point to another. The shock can sustain the detonation in two ways. Firstly, if the kinetics of the dissociation is strongly pressure dependent, the reaction rate can be enhanced in the high-pressure domain behind the shock front. Secondly, the shock can have a more direct effect because, inside the shock front, the molecular lattice suffers very violent distortions which are responsible for strong forces acting on the molecules, which can assist, or even cause, their dissociation. The molecular dynamics results suggest that, in a solid phase, this second mechanism is the dominant one, in agreement with the conclusions reached by Dremin and co-worker and Walker from many experimental studies [3, 4]. Although the first mechanism could be introduced in the model by using a kinetic constant K which is a function of the atomic distance $R_i - R_{i-1}$, we have chosen to include only the second mechanism in the model to reduce the number of free parameters and to allow for some analytical analysis. Consequently, equation (8) is modified by replacing the diffusion term by $-D(R_i - R_{i-1})/a$ which introduces a direct effect of the shock front on the reaction rate. The coupled equations for the atomic motions and the chemical reaction are consequently written as

$$m \frac{d^2 R_i}{dt^2} = G(R_{i+1} - 2R_i + R_{i-1}) + A [(R_{i+1} - R_i)^2 - (R_i - R_{i-1})^2] - \alpha \frac{\Phi_i - \Phi_{i-1}}{a} - \gamma \frac{dR_i}{dt} \tag{10a}$$

$$\frac{d\Phi_i}{dt} = -D \frac{R_i - R_{i-1}}{a} + K \Phi_i (\eta - \Phi_i) (\Phi_i - 1). \tag{10b}$$

These equations can also be written in terms of the relative atomic displacements $U_i = R_i - R_{i-1}$ as

$$m \frac{d^2 U_i}{dt^2} = G(U_{i+1} - 2U_i + U_{i-1}) + A [U_{i+1}^2 - 2U_i^2 + U_{i-1}^2] - \alpha \frac{\Phi_i - 2\Phi_{i-1} + \Phi_{i-2}}{a} - \gamma \frac{dR_i}{dt} \tag{11a}$$

$$\frac{d\Phi_i}{dt} = -D \frac{U_i}{a} + K \Phi_i (\eta - \Phi_i) (\Phi_i - 1) \tag{11b}$$

3. Properties of the model

3.1. Limit of slow reaction kinetics

In the continuum limit, equations (11a, b) become

$$u_{tt} - c_0^2 u_{xx} - p(u^2)_{xx} - hu_{xxxx} + \frac{\gamma}{m} u_t = -\frac{\alpha}{m} \phi_{xx} \tag{12a}$$

$$u = -\frac{1}{D} \phi_t + \frac{K}{D} \phi (\eta - \phi) (\phi - 1). \tag{12b}$$

In these equations, only the leading derivatives in ϕ have been conserved. In spite of this simplification, we have not been able to solve this coupled system of equations in the general case, but a solution can be obtained in the limit $K/D \ll 1$, which amounts to assuming that the kinetics is slow and that the chemical dissociations are completely driven by the shock. With these approximations, equation (12b) gives $u \simeq D^{-1} \phi_t$, and, in a steady detonation

propagating at speed v , where the solution has a permanent profile, $\phi_x = -v\phi_t$ allows us to eliminate ϕ from equation (12a) to obtain

$$v^2 u_{xx} - c_0^2 u_{xx} - p(u^2)_{xx} - hu_{xxxx} + \frac{\gamma}{m} u_t = -\frac{\alpha D}{mv} u_x + \frac{\gamma v}{m} u_x. \quad (13)$$

If the velocity v is such that

$$v = v_c = \sqrt{\frac{\alpha D}{\gamma}} \quad (14)$$

the right-hand side vanishes and equation (13) reduces to the Boussinesq equation written for a permanent profile solution, which has a soliton solution. Therefore for this particular velocity v_c , the system sustains a detonation wave which combines a shock and a chemical reaction propagating at the same speed. The stability of this solution can be analysed by considering the case of a detonation propagating at a velocity close, but not equal, to v_c . Let us assume $v = v_c(1 + \sigma)$, with $\sigma \ll 1$. Using again $u \simeq D^{-1}\phi_t$ from equation (12b), equation (12a) becomes

$$u_{tt} - c_0^2 u_{xx} - p(u^2)_{xx} - hu_{xxxx} = 2\sigma \left(\frac{\alpha D}{v_c} \right) u_x \quad (15)$$

where the permanent profile assumption has been used for u in the RHS which is a small perturbative term, and the calculations are limited to order unity in σ .

In order to study the effect of the perturbation due to the non-vanishing RHS of equation (15), it is convenient to consider the limit where it reduces to a Korteweg de Vries equation to take advantage of the well known perturbation methods for KDV [12]. This is accomplished by changing to the frame moving at the sound speed c_0 by the introduction of the variables $\xi = x - c_0 t$ and $\tau = t$. In this frame the time evolution of the solution can be assumed to be small enough so that the second-order time derivative in τ can be neglected. With these assumptions, and after one space integration with vanishing boundary conditions at infinity adapted to a solitary wave, equation (15) becomes

$$u_\tau - \frac{|p|}{2c_0} (u^2)_\xi + \frac{h}{2c_0} u_{\xi\xi\xi} = -\frac{\sigma}{c_0} \frac{\alpha D}{v} u. \quad (16)$$

For $\sigma > 0$ ($v > v_c$), a perturbation of the KDV equation proportional to u causes an exponential decay of the amplitude and velocity of the soliton [12], while for $\sigma < 0$ ($v < v_c$) the perturbation causes an exponential growth of its amplitude and speed. Consequently, the calculation indicates that a detonation propagating at velocity v_c is *stable*. A faster detonation is expected to slow down gradually to v_c where the perturbation vanishes, while a slower one should accelerate to v_c .

Of course these conclusions are valid only for a small range of velocities around v_c , and they are derived in the continuum limit, which is only a rough approximation for a detonation wave. Therefore they must be checked directly by numerical calculations. This has been done by solving the discrete set of equations (11a, b) with an initial condition which is obtained from the continuum limit approximation. The solution for u is obtained from equation (13) and ϕ is derived from equation (9) which has qualitatively the correct shape. Figure 1 shows the time evolution of the velocity of the detonation wave for various initial velocities v . The model parameters used in this calculation are $K = 0.01 \text{ TU}^{-1}$, $D = 1 \text{ TU}^{-1}$, $\eta = 0.25$, $\alpha = 0.02 \text{ eV}$, $\gamma = 0.01 \text{ amu TU}^{-1}$, so that the approximation $K/D \ll 1$ is verified (our time-unit 'TU' is equal to 10^{-14} s and 'amu' designates the atomic mass unit). The characteristic velocity corresponding to these parameters is $v_c = 1.414 \text{ \AA TU}^{-1}$. Since the initial condition is derived in the continuum limit, it is not an exact solution of the

discrete equations of motions and it emits transients which propagate at the speed of sound and thus stay behind the detonation wave. To check that the detonation wave reaches a permanent profile steady state, these transients are removed from the solution when they are sufficiently separated from the front. Then, when the initial speed is not close to v_c , the detonation wave emits other small-amplitude waves as it speeds up or slows down towards v_c . After some time the solution is 'cleaned' a second time by removing these small-amplitude waves and we follow its evolution to check its stability. Figure 1 shows that all the initial conditions with initial velocities in the domain $1.01 \leq v \leq 1.60$ converge to a final velocity $v_f = 1.36 \text{ \AA TU}^{-1}$ which is in very good agreement with the theoretical velocity v_c . This result shows that our simple detonation model has a well defined detonation speed, which does not depend on the initial condition, as found in experiments. A better test of the stability of the solution is to measure the energy of the detonation wave in a region which contains the shock and reaction fronts and propagates with them. Figure 2 shows the time evolution of the energy of the 100 cells which contain the fronts for the various initial conditions shown in figure 1. It demonstrates the very good stability of the detonation over long periods. Other parameter sets confirm the validity of the analytical analysis to determine the detonation velocity to a good accuracy. The theoretical values overestimate slightly the equilibrium values found in the numerical calculations because they do not take into account properly the effects of the chemical kinetics which is simply ignored in our approximation $K/D \ll 1$.

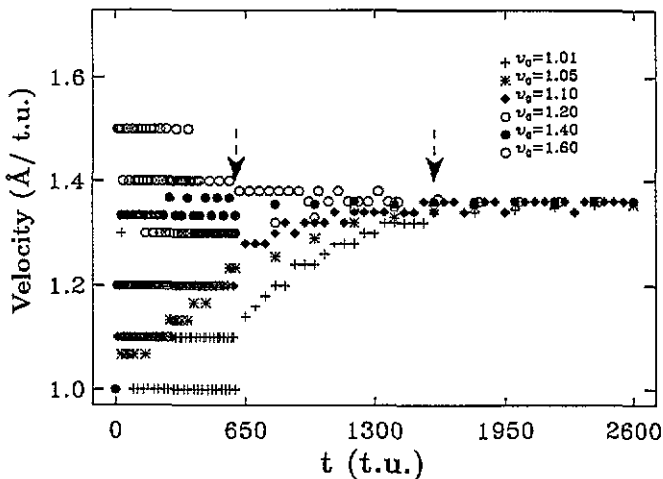


Figure 1. Time evolution of the velocity of a detonation wave in the limit $K/D \ll 1$ for various values of the initial velocity. The theoretical velocity of the stable detonation speed is $v_c = 1.414 \text{ \AA TU}^{-1}$, and the initial velocity has been varied from $v = 1.0$ to $v = 1.6$. The arrows indicate the times at which the transients emitted by the initial condition have been eliminated.

3.2. General case

Although these results are interesting they do not really describe the interplay of the chemical reaction and shock in the detonation because, in order to allow analytical calculations, they have been obtained with the assumption $K/D \ll 1$ which means that the reaction is dominated by shock-induced dissociations. More interesting properties can be found if one drops this assumption, but we have to rely completely on numerical calculations. The

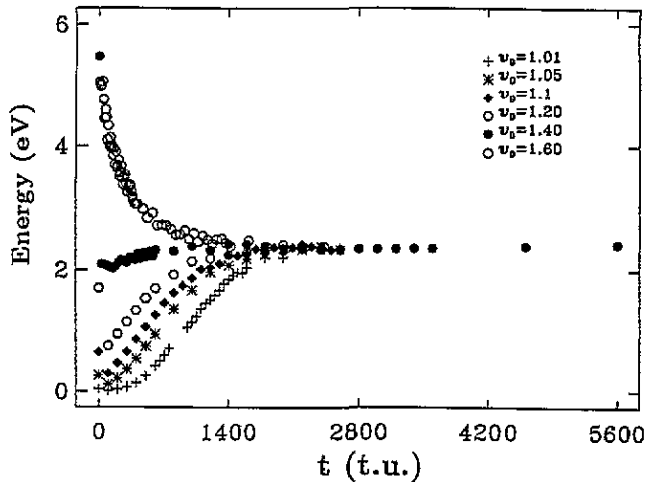


Figure 2. Time evolution of the energy of a domain of 100 cells containing the shock and reaction fronts and propagating with them.

analytical results are only used to derive approximate initial conditions for the numerical studies in which we observe the structure of the detonation wave which emerges from these initial conditions. We have performed a series of numerical calculations with $K = 1.0 \text{ TU}^{-1}$ (a value 100 times larger than before) and various values of D in the range $0.125 \leq D \leq 1.0 \text{ TU}^{-1}$ so that, now, the chemical kinetics and the shock-induced reaction play similar roles in the detonation process. For each value of D , several values of the initial velocity v have been tested. Figure 3 summarizes the results.

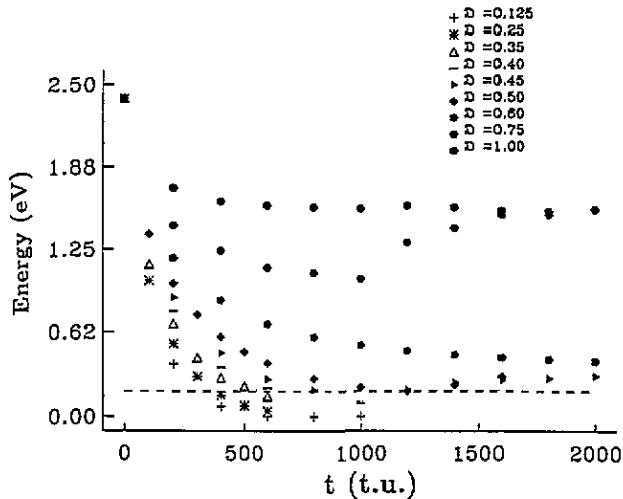


Figure 3. Time evolution of the energy of the detonation front for $K = 1 \text{ TU}^{-1}$ and different values of D . The dotted line indicates the energy threshold for the initiation of a stable detonation.

When D is too small ($D < 0.4 \text{ TU}^{-1}$), the coupling between the shock and the chemical reaction is not sufficient to maintain a steady detonation, whatever the initial velocity. In this case the compound is not an explosive material. Any detonation that could be initiated

by a very strong shock dies out. For larger D there is a minimal initial velocity to create a steady detonation. We recover here the existence of a detonation threshold observed in experiments and in numerical calculations. If v is below the threshold, the reaction lags behind the shock and finally stops propagating, and then a simple shock wave subsists. The thresholds can be expressed as a minimum energy in the domain around the shock, and it is shown as a dotted line in figure 3.

When the initial condition is over this threshold, a steady detonation is observed, but it is interesting to notice that, when D varies, we find *two well defined detonation regimes* instead of a continuous variation of the properties of the detonation as one could have expected from a continuous variation of D . Figure 3 shows that, when D increases over the value $D = 0.60 \text{ TU}^{-1}$, the detonation switches from a low-energy and low-speed regime to a high-energy high-speed regime. This is an unexpected result since nothing is built into the model to generate such a behaviour, and it is particularly interesting because the same property was found in our last molecular dynamics results with an improved model designed to study the role of crystal inhomogeneities [8]. In these simulations of a shock-induced detonation in a homogeneous sample, we found *two very different detonation regimes* depending on the characteristics of the impact. For a 'slow impact' during which the average acceleration of the shocked atoms is below some threshold A_c , the detonation propagates with a speed of about 7.5 km s^{-1} which is a characteristic of the material and not of the initial impact. We called this regime the slow-detonation regime. A very fast impact generates a steady detonation which propagates with an extremely high speed of about 23 km s^{-1} . We called this regime the fast-detonation regime. The slow- and fast-detonation regimes are qualitatively very different. In the fast regime, the induction zone which separates the shock front from the reaction front is very narrow (one or two cells only) and the crystal structure is still rather well preserved in the reaction zone so that the molecular dissociations followed by the energy release occur in a coherent manner close to the shock front. Only a small part of the chemical energy is lost in disordered motions that do not sustain the detonation. This explains the extremely high detonation speed which is however a characteristic of the material because the same speed is obtained for all impacts exceeding the threshold A_c . The induction zone is much bigger in the slow detonation regime than in the fast regime. Moreover, in the reaction zone of the slow regime, the crystal structure is so distorted that the molecules are randomly oriented. Thus the energy release occurs in an incoherent way which is not as efficient as in the fast regime to sustain the propagation of the shock.

Although there is not a direct connection between the two-dimensional molecular dynamics simulations and our one-dimensional approach, it is remarkable to recover the existence of the two detonation regimes from a simple model. Here the separation between the two regimes is obtained by changing D , i.e. the coupling between the shock and the reaction rather than the amplitude of the initial shock as in the molecular dynamics simulations. This difference is due to the nature of the initial condition that we use in the one-dimensional model. Instead of an initiation by a shock at one end of the lattice which allows the system to adjust itself to the steady detonation state, we impose an initial condition which derives from an approximate analytical solution that puts more constraints on the initial state because it is applied to the whole system. However the similarity between the molecular dynamics simulations and the one-dimensional model is strong because the small distance between the shock and reaction fronts found in the fast regime of the molecular dynamics simulations is associated with a strong coupling between the two fronts, which corresponds to the large- D case in the one-dimensional model, while the inefficient energy transfer between the shock and the reaction in the slow regime corresponds to a small D

value in the model.

4. Conclusion

The model that we have presented here has been specially adapted to the case of solid phase detonations, and therefore it is fundamentally different from the usual models for gases or fluids. The mechanical part considers a lattice which is described by a hyperbolic equation, which includes the non-linearities which are excited in the high-speed shock wave of a detonation, rather than by an equation for heat diffusion or a hydrodynamic equation. Although the continuum limit is used in the analytical calculations, the full discreteness is conserved in the numerical treatment of the model. This aspect is important because *all* the molecular dynamics simulations [2, 3, 5–8] although they have used extremely different models from simple atom-and-springs systems to sophisticated three-body potentials to reproduce accurately the chemical reactions, have concluded that the detonation front is extremely narrow on the molecular scale. In the chemical part of our model, the diffusion of the species has been removed since it does not occur appreciably in a solid, and replaced by a coupling with the atomic displacements caused by the shock.

In spite of its simplicity, the model reproduces the general properties of a detonation like the existence of a characteristic speed or a detonation threshold. Moreover it is interesting to notice that it gives also a non-trivial result found in molecular dynamics simulations: the existence of a fast high-energy and of a slow low-energy regime for the detonation. Due to the fundamental difference between the two approaches, it is hard to believe that this is only a coincidence. Certainly these two regimes deserve further investigations, from both the experimental and the theoretical points of view.

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