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14. ABSTRACT Impact and penetration tests were conducted by the Air Force Research Laboratories (AFRL/MN), at striking velocities in the range of 1200 to 1500 meters per second. Steel projectiles were impacted into selected concrete targets. At these striking velocities, the impacting steel projectiles were subjected to a significant mass loss from the nose region. Changes of the nose shape, deposition of melted steel on the nose and the shank of the projectile were observed. In parallel, the Institute of Physics of the Earth of Russian Academy of Sciences (IPE RAS) has reported on the study of the high-speed impact and penetration of metallic projectiles into sand targets. Many interesting observations have been reported from these experiments. Projectiles experienced a significant amount of heat. Phase transitions including melting have been observed in the projectiles. Melting was observed in the nose region.					
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THERMOMECHANICS OF IMPACT & PENETRATION

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INTRODUCTION/MOTIVATION: Impact and penetration tests were conducted by the Air Force Research Laboratories (AFRL/MN), at striking velocities in the range of 1200 to 1500 meters per second. Steel projectiles were impacted into selected concrete targets. At these striking velocities, the impacting steel projectiles were subjected to a significant mass loss from the nose region. Changes of the nose shape, deposition of melted steel on the nose and the shank of the projectile were observed. Even when the impact was normal to the surface, the trajectory of the projectile, through the target, deviated from the intended straight trajectory. These observations were the motivations for this project.:

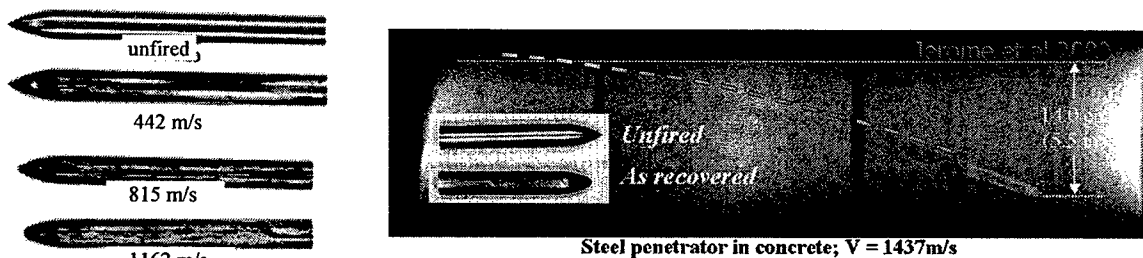


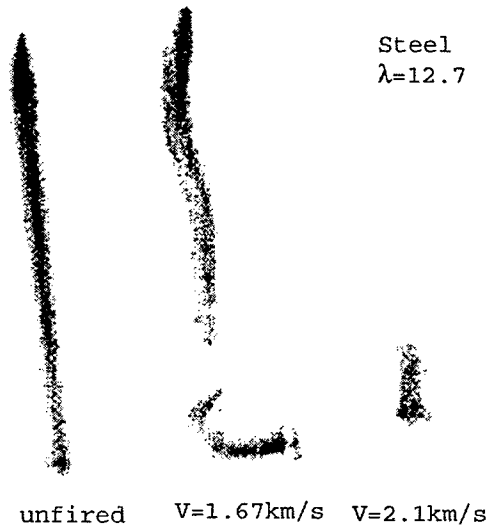
Figure 1. Nose erosion of the 20.3 mm diameter, 4340 Rc 45 projectiles striking into concrete targets (Frew et al. 1998), and deviation of penetration by Jerome et al. 2000.

In parallel, the Institute of Physics of the Earth of Russian Academy of Sciences (IPE RAS) has reported on the study of the high-speed impact and penetration of metallic projectiles into sand targets¹. The striking velocities were in the range of 4000 meters per second. An electro-discharge launcher (EDL) was used as the accelerator in these studies. The materials selected for projectiles included steel and a tungsten alloy (WNiFe). The projectile aspect ratio ($\lambda=L/d$, where L – projectile length, d – projectile diameter) varied from 1 (ball) up to 12 (long rod). The dry sand was used as the target. The density of sand was $1,820 \text{ kg/m}^3$. The target also indicated some void contents in the sand. The solid density of quartz is around $2,200 \text{ kg/m}^3$. A limited number of tests were also conducted with wet sand targets to compare the results with the penetration results into dry sand targets.

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¹ Savvateev, AF, Budin, AV, Kolikov, VA, and Rutberg, PhG. High-speed penetration into sand. Int J Impact Engng 26 (2001), 675 – 681.

Many interesting observations have been reported from these experiments. Projectiles experienced a significant amount of heat. Phase transitions including melting have been observed in the projectiles (Figure 2a-3, 2b-2 and 3, 2c-2 and 3). Melting was observed in the nose region. A critical striking velocity was identified. When the striking velocity of the projectile exceeded this critical velocity, a significant amount of melting of the projectile took place. In some cases, "a projectile breakup" was also observed. For large aspect ratios (e.g. $\lambda=12$), projectiles bent (or buckled)..



OBJECTIVES

The objectives are to understand the impact and penetration mechanisms of metallic projectiles into granular targets, at high striking velocities, formulate appropriate constitutive models, and solve selected problems by using these models, appropriate equations of conservation and failure criteria, explain the observed mass loss from the nose region, changes of the nose shape, deposition of melted steel on the surface of the recovered projectile, the heat affected zone beneath the surface of the projectile and the deviation of the trajectory from the intended trajectory, design tests to validate key results by tests, develop simplified models similar to the cavity expansion theory, and discuss modification of the analysis to other target media like sand, concrete and soil

To develop multi-scale computations of the impact and penetration, the objective also includes a development of techniques to determine the equations of state of projectile materials and high-strain-rate phase transitions under conditions of high pressures (or stresses) and high temperatures. The next step is to determine the parameters of the constitutive models by experimental results or ab initio techniques. Following the development of the constitutive relations and conservation equations, the next objective is to study the interaction of different targets with the projectile during high-speed impact and penetration. This leads to the study of selected problems numerically by multi-scale computations that can combine quantum mechanics scales, molecular dynamic scales and

continuum mechanics scales to provide an accurate understanding of the observed phenomena.

RESEARCH TASKS OF THIS PROJECT

- ◆ Observation of recovered projectile
- ◆ Formulation of penetration mechanisms
- ◆ Formulation of constitutive equations to reflect the observations, including stress-induced phase changes, and plastic work and friction effect to heat the projectile
- ◆ Solutions of selected problems (Applications of nonequilibrium thermodynamic model)
- ◆ A simplified model, using a combination of cavity expansion theory, deformable projectile and modification of Walker model to explain nose erosion and resulting penetration path. (Modification of cavity expansion theories)
- ◆ Ab Initio Models to Predict the parameters of the constitutive models (preliminary work only)
- ◆ Multiscale Numerical Simulations (preliminary work)

PROGRESS

Time-Dependent Penetration Path of Deformable Projectile into Selected Targets

In the last report, we discussed analysis of recovered projectiles, the possible penetration mechanism with dislocation pile-up behind the shock wave and a 3-dimensional model, for phase changes, in the frameworks of non-equilibrium thermodynamics and a mixture theory. A dislocation based plasticity model was also developed for the impact and penetration analysis. Numerical solutions were presented for selected cases. In this report, the formulation of a simplified model and solutions are discussed. This is followed by a discussion of the preliminary work on multiscale computations.

In 1967, Tate² developed a model for a deformable long-rod penetration by using a hydrodynamic approximation. Prior to this work, most penetration mechanics models were based rigid projectiles. The Tate's model can determine the time history of penetration. The projectile and the target were both treated as fluids with modifications.. The variation of the penetration velocity in Tate's model shows significant differences from experimental observation.. Later, Walker modified Tate's model by integrating the 3 dimensional equations along the centerline of the projectile. In this project, we extend the Tate and Walker's model and combine it with the cavity expansion model by Hanagud and Ross³ to consider a conical nose-shaped projectile penetrating into specific targets. The modification from Walker's model consists of the two-dimensional velocity and stress profiles (r, z), which can be obtained from previous numerical simulations. Besides the elastic and plastic regions in the projectile, phase transition region with the

² A Tate, J. Mech. Phys. Solids, V15, 287(1967)

³ Hanagud, S., and Ross, B., "Large deformation, deep penetration theory for a compressible strain-hardening target material," AIAA J., v. 9, n. 5, 1971, pp. 905-911.

plastic flow near the nose tip is incorporated in the model by using results by Lu and Hanagud⁴. In this model, by knowing the initial impact velocity, the equation of linear momentum balance equation is explicitly integrated through the centerline of the projectile and through the radius of the conical projectile to obtain the time variation of the penetration velocity. In other words, we have modified Walker's model and cavity expansion theory to include the effects of phase transition.

A 1-D MODEL WITH CHANGING CROSS-SECTION AREA IN THE NOSE REGION

As a first step to understand blunting of the nose tip and the initiation of phase transition, the equations are simplified to obtain a 1D model with changing cross-section area in the nose region. Through the analysis of the plastic region by using shock wave conditions and the resistant force by cavity expansion theory, we formulated the equations for the time-dependent penetration path by integrating the 1D mass conservation and linear momentum balance equation for plastic region. At the shock wave front from elastic region to plastic region, Hugoniot jump conditions are used. After obtaining all the relevant equations, we used a perturbation method to find the solution. First, we consider the projectile to attain a locking density ρ_{lp} at the nose tip and change steadily entire plastic region. Then we analyze the first order of perturbation with conditions $\rho(z, t) = \rho_{lp}$. Secondly, we consider the particle velocity attains $V_A(t)$ at the nose tip and change steadily to a locking velocity in the plastic region $v_z(z, t) = V_A(t)$.

Perturbation based on a locked density in the plastic region

The final equation for time-dependent penetration velocity V_A is

$$\rho_{lp} \left\{ -\frac{1}{5}(z_B - z_A)(\dot{V}_B - \dot{V}_A) - \frac{2}{3}[-V_A(z_B - z_A) + z_A c_p](V_B - V_A) + (z_B - z_A)\dot{V}_A \right\} \\ = \rho_e \frac{(V_A - V_e)^2}{1 - \alpha} + P_0 + \frac{2}{3}Y_p - \xi P^I(t)$$

Perturbation based on a locked particle velocity in the plastic region

The final equations consist of two ODEs governing the penetrating velocity V_A and a density ratio α .

$$\dot{V}_A = \frac{\rho_e(1 - \alpha)^{-1}(V_A - V_e)^2 + \sigma_e - \xi P_s - \xi \rho_{lp} B_2 V_A^2}{\rho_e(1 - \alpha)^{-1} \int_0^t (V_e - V_A) dt + \xi \rho_{lp} B_1 d} \\ \dot{\alpha} = \frac{(1 - \alpha)[(1 + 3\alpha)V_A - 4\alpha V_e]}{3 \int_0^t (V_e - V_A) dt}$$

Phase Transition in the Plastic Region

We assume a linear variation of the pressure with respect to z direction in the plastic region. The rate of work done by the shock compression in the plastic region is given by

⁴ Xia Lu & S. Hanagud, Nonequilibrium Polycrystalline Solids, Technical report, Georgia

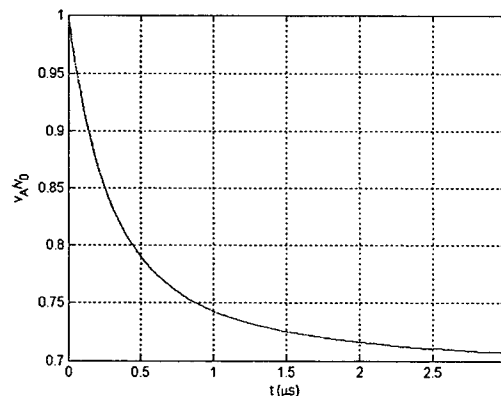


Figure 2. Time variations of the penetration velocity $v_A(t)$ for steel projectile into ($Mg_{0.8}Fe_{0.2}SiO_3$) Perovskite target.

$\dot{W}(z, t) = P(z, t)\dot{\alpha}$. If we assume that only two phases can coexist, the mass fraction for the second phase is given by γ , and the mass fraction for the first phase is $(1 - \gamma)$.

$$\rho\dot{\gamma} = \frac{1-\gamma}{\Delta G_{1 \rightarrow 2}} \dot{W}$$

For example studies, we considered a hard target with material constants for $\rho_{t0} = 4190 \text{ kg/m}^3$, $\rho_{tip} = 5500 \text{ kg/m}^3$ (selected), $Y^t = 60 \text{ MPa}$, $E^t = 260.09 \text{ GPa}$ (Young's modulus), $E^t = 13 \text{ GPa}$ (strain hardening modulus). In the following simulations, the initial impact velocity is 1500 m/sec. The time-dependent penetrating velocity is shown in Figure 14. Phase transitions are calculated. The mass fraction of phase 2 as a function of z and t is presented in Figure 3a, time variations of mass fraction of phase 2 at locations $z=z_A$ and $z_A - 0.5\text{mm}$ are presented in Figure 3b; and the profiles of mass fraction of phase 2 at particular times $t = 0.055$ and $3 \mu\text{s}$ are presented in Figure 3c.

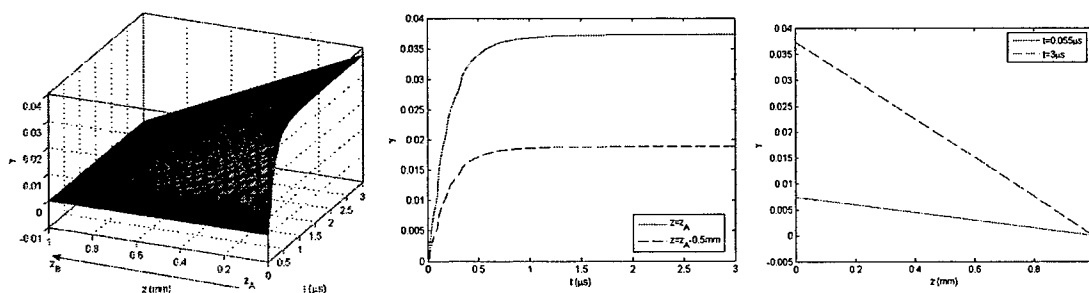


Figure 3. The time variations of the phase transition profile for steel projectile (a) Mass fraction of phase 2 as a function of z and t ; (b) Time variations of mass fraction of phase 2 at locations $z=z_A$ and $z_A - 0.5\text{mm}$; and (c) Profile of mass fraction of phase 2 at particular times $t = 0.055$ and $3 \mu\text{s}$.

MULTISCALE COMPUTATIONS

A multiscale computation by a combination of the integration of *ab initio* related techniques (quasistatic or dynamic), molecular dynamics and continuum numerical schemes (finite element or finite difference) can be used to directly study impact and penetration events of metal projectile into sand targets. In the past, QM methods have been combined with molecular dynamics (MM) ^{5,6,7,8,9,10}, in the form of Born-Oppenheimer molecular dynamics¹¹ or Car-Parrinello Molecular dynamics¹². On the other hand, MM has been combined with continuum mechanics^{13,14,15,16,17}. In this project, we use a new concept to understand the impact and penetration of metallic projectiles

5 Monard, et al. Acc. Chem. Res. 1999, 32, 904.

6 Warshel and Levitt, J. Mol. Biol.

7 Field, Bash and Karplus, J. Comp. Chem.

8 Bylaska, E.J., Rustad, J.R., and Dupuis, M. Environmental Dynamics and Simulation 1999 Annual Report.

9 Rustad, J.R., Bylaska, E.J., Dixon, D.A., Felmy, A.R., and Rosso, K.M. Environ. Dyn. Simul. 1999 Annual Report.

10 Blöchl, P.E., Phys. Rev. B, 1994, 50(24), 17953 – 17979.

11 Hutter, Lecture notes. Introduction to *ab initio* molecular dynamics. 2002.

12 Marx and Hutter, NIC Series, 2000, 1, 301 – 449.

13 Hoover et al. Cout. Phys., 1992, 6.

14 Kohloff et al. Phil. Mag. A, 1991, 64.

15 Rudd and Broughton. Phys. Rev. B, 1998, 58.

16 Tadmor, Phillips and Ortiz. Langmuir, 1996, 12, 4529.

17 Park, Karpov and Liu.

into concrete and sand targets, which is by a combination of QM/MM/continuum scales through incorporating the ab initio (quantum mechanics based analysis) into molecular dynamics, and molecular dynamic into continuum based computational procedure through multi scale computational procedures. For continuum level, we use the constitutive models for projectiles and sand targets developed in the framework of nonequilibrium thermodynamics. This new concept has the potential to provide an understanding from first principles and minimize many costly experiments. .

In the QM/MM/continuum approach, two types of boundary regions have to be considered (Figure 5): one is the QM/MM boundary, and the other is MM/continuum boundary. For the first type of boundary, two methods are used to adjust cross-interaction of QM and MM: First, a frozen QM core approximation is used In the second method the ab initio QM/MM approach where Coulomb interaction is calculated accurately. For the second type of the boundary, a mesh refining method^{13,14} is used. Only preliminary work has been done in this area. The QM/MM/continuum approach can yield the localized complicated phenomena, which involves multiple length and time scales. In comparison to the ab initio studies, we will focus In future) on the dynamic shock effects on the interaction between the projectile and concrete or sand. In this approach, the dynamic effects (or kinetic energy effects) will be automatically to different scales.

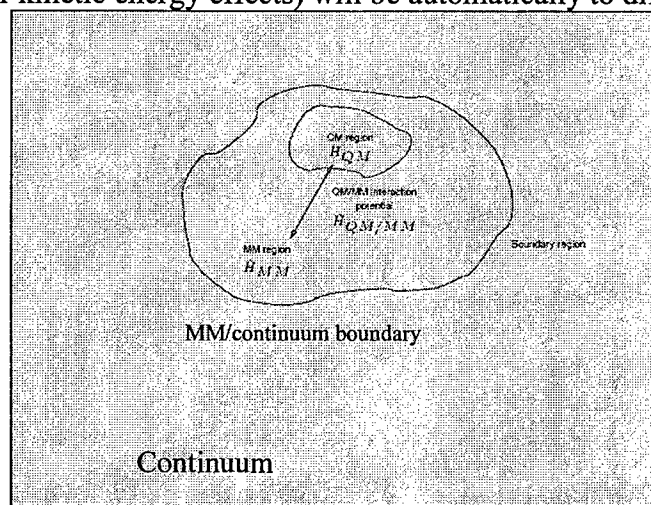


Figure 4. QM/MM/Continuum Approach.

AB INITIO (FIRST PRINCIPLES OR QUANTUM MECHANICS) BASED STUDIES

As a first step of multiscale modeling, we initiated on employing ab initio techniques to obtain material constants and modifying the abinitio molecular dynamic equations to account for increasing temperature and dynamic loading. The ab initio techniques to be employed is based on the density functional theory (DFT), using local density approximation (LDA) or generalized gradient approximations (GGA) for exchange-correlation potentials, and projector augmented wave (PAW) methods for interaction between ions and electrons. The electronic and lattice thermal effects are be included by using electronic band structure calculations and phonon analysis, respectively. Boltzmann statistics and Fermi-Dirac statistics are used to bridge the atomistic level to continuum level.

Currently, we are working on the equations of state of iron/ steel, with phase transitions, including melting, at high stresses (pressures) and high temperatures. Preliminary results have been developed in the area of ABMD calculations.

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