2.2 SHOCK WAVE PHYSICS RELATED ACTIVITIES

Gas gun facility at BARC

For studying the response of material to high stress and strain rates a gas gun facility has been developed at our laboratory (Fig.). The gun is capable of accelerating the projectile up to the velocity of 1 km/s, and generating the pressure of 40 GPa in the target material.

The gun has three main parts: breech, barrel and target catcher system. The breech contains a gas at high pressure and breech opening mechanism provides within a few milliseconds the unrestricted flow of gas behind the projectile. The barrel is a 3 meter long high tensile strength steel pipe with outer diameter of 114 mm and inner diameter of 63 mm. A straight slot, 3 mm wide and 1.9 mm deep, has been machined in the internal surface of the barrel. Also, a 2.5 mm long brass key with the same cross-sectional dimensions as that of slot is fitted to the projectile. This key is guided through the slot during the acceleration of the projectile and facilitates the impacts of inclined parallel plates for compression-shear experiments. The target catcher system consists of two sections separated by a thick mylar diaphragm. The first section (target chamber) permanently mounted to the muzzle end of the barrel is evacuated to 10 millitorr using a rotary and roots vacuum pumps. The second section is movable and contains the projectile and target stopping mechanism. The firing of the projectile is done with a remote control unit. The amplitude of the stress pulse in the target depends on the velocity of the impactor. The duration of shock (a few μs) in the target is determined by the impactor thickness (a few mm) and impedance of the impactor and target material. The projectile can be accelerated to the desired velocity by suitably selecting the breech pressure. Diagnostic techniques like electrical pins, manganin gauge technique, self shorting pins, ionization pins and optical pins are used for measurement of projectile velocity, shock pressure and shock velocity. A series of four pairs of electrical pins are used to measure the projectile velocity just before the impact. The manganin gauge technique is used for measurement of time resolved stress profile and shock velocity in the shock-loaded target. The self-shorting pins, ionization pins and optical pins are used to measure the shock velocity in the target. For investigation of shock induced structural phase transitions in powder or brittle sample a special capsule (recovery fixture) is used for holding the sample. In these experiments, termed as recovery experiments, shock pressure in the sample is determined indirectly from the hydrodynamic code in conjunction with measured projectile velocity. The sample recovered after unloading from peak shock pressure is characterized through X-ray diffraction and Raman measurements for any irreversible phase transition.


Theoretical Investigation of Pressure Induced Phase Transition in Ti at High Pressures

The group IV B elements are expected to undergo s-d electron transfer under pressure and, thus, mimic the transformation sequence $\alpha \rightarrow \omega \rightarrow \beta$ shown by these elements with increasing number of d electrons on alloying with d-electron rich neighbors. This structural sequence under pressure is well established for Zr and Hf. However, Ti metal has been reported to undergo a transition from hexagonal phase (ω) to an orthorhombic phase (distorted hcp, γ-phase) at 116 GPa,
whereas there are also reports that titanium undergoes a transition to the $\gamma$-phase from the $\omega$-phase. To resolve this we have carried out total energy calculations employing the FP-LAPW method to examine the stability of the $\gamma$ and $\delta$ phase with respect to the $\omega$ and $\beta$ structures. Our analysis predicts at 0 K the $\omega$-phase transforms to $\beta$-phase via intermediate $\gamma$-phase, whereas at 300 K the $\omega$-phase transforms to $\beta$ structure directly and the $\gamma$-phase becomes most competing metastable structure in the pressure range of $\beta$-phase stability. The $\delta$-phase, however, is not at all stable at any compression. It suggests that the $\gamma$-phase observed in the experiments is a metastable phase that could be formed due to the shear stresses present in the experiments and the $\omega \rightarrow \gamma$ structural transition does not represent the phenomenon expected under hydrostatic conditions.

**Ab-initio Calculations for Comparison of Hardness of Osmium and Diamond**

On the basis of the high-pressure diamond anvil cell experiments on Os metal, Cynn et al. have reported that the bulk modulus of this metal is 462 GPa, higher than that of diamond (445 GPa), the hardest material known so far. Based on this they concluded that it has lower compressibility than diamond. We have reanalyzed the experimental data of Cynn et al and found that the bulk modulus of Os (434 GPa) and diamond are close to each other, implying that Os metal is as incompressible as the diamond but not more. We also, performed the first principles total energy calculations on Os and diamond using full potential linearised augmented plane wave method under both Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA). For LDA calculation the value of $B_0$ estimated from Birch–Murnaghan fit is 461 GPa for
osmium and 464 GPa for diamond. From GGA calculations, this parameter is estimated as 436 GPa and 432 GPa, respectively, for the two elements. Thus, we find the theoretical values of $B_0$ for Os are comparable to the corresponding values of diamond for both LDA and GGA calculations.

**TEM Study on Shock Compressed Zr-20 Nb Alloy**

The TEM study on shock compressed Zr-20 %Nb alloy have been done in collaboration with Materials Science Division, BARC. This alloy having bcc ($\beta$) structure at ambient condition was subjected to a peak shock pressure of 15 GPa in a 63 mm bore gas gun at our laboratory. The electron diffraction measurements of the retrieved sample confirmed the $\beta \rightarrow \omega$ transformation. The $\beta \rightarrow \omega$ transformation has been observed for the first time in an alloy under shock compression. The $\omega$-phase so formed has plate shape morphology and orientation relationship have been found same as that observed in $\omega$-phase formed on thermal treatment of the alloy. The formation of the $\omega$-phase has been explained on the basis of shear and shuffle of atoms on $\{112\}\beta$ planes.


The shock compression experiments generate not only the compressive high pressures but also high tensile stresses. Sophisticated diagnostic techniques like VISAR and ORIVIS, used recently to measure such tensile stresses, throw light on the material behavior in the negative pressure regimes. We have determined the ideal spall strength ($\sigma_s$) and also, the equation of state (EOS) in the negative pressure region for Mo and group IV B metals (Ti, Zr and Hf) from first principles total energy calculations using full-potential linearised augmented plane wave (FP-LAPW) method (WIEN97 Package). For Mo, we have calculated the ideal tensile strength ($\sigma_T$) and the elastic constants also. The $\sigma_s$ is calculated using uni-axial strain i.e. without allowing the Poison contraction, however for $\sigma_T$ the Poison contraction was also allowed.

The calculated $\sigma_s$ along [1 0 0] for Mo is 41 GPa as compared to the experimental value of 16.5 GPa measured after unloading the sample from peak pressure of 75 GPa (strain rate ~3X10^7/s). Our calculated $\sigma_s$ value is 23 GPa. The calculated equilibrium volume is 15.96 (Å)^3/atom, elastic constants $c_{11}$, $c_{12}$, $c_{44}$ are 439, 175, 100 GPa, and $B_0$, $Y(1 0 0)$, $Y(111)$ are 272, 339, 266 GPa, respectively.

For Ti, Zr and Hf we have determined $\sigma_s$ along [0001] direction for hcp ($\alpha$) and three atom hexagonal phase ($\omega$). The calculated $\sigma_s$ for $\alpha$ phase of Ti, Zr and Hf is 22, 18 and 20 GPa, and for the $\omega$ phase is 24.2, 19.5 and 23.6 GPa, respectively. The $\omega$ phase is found to be harder than $\alpha$ phase in agreement with available experimental results. The trend in the group IV B indicates that $\sigma_s$ for Ti is largest followed by Hf and then Zr for both $\alpha$ and $\omega$ structures. The theoretical $\sigma_s$ for Ti is much lower than the experimental $\sigma_s$ value.
higher than \sim 4.2 \text{ GPa} \text{ measured at strain rates of} \sim 10^6/\text{s}. \text{The bulk modulus of 110, 96 and 115 GPa, respectively for Ti, Zr and Hf, determined from the theoretical EOS in the negative pressure region, are in good agreement with experiments.}

The theoretical value of the \( \sigma \text{s} \) for Mo and Ti are higher than the available experimental values. This discrepancy could be associated with the material defects, which dominantly control the spalling at such strain rates. For determination of ideal \( \sigma \text{s} \), experiment should be performed at still higher stresses (and higher strain rates) to minimize the effects of material defects.

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**K.D. Joshi and Satish C. Gupta, Joint-AIRAPT International Conference on High Pressure Science and Technology, 2005.**

**K.D. Joshi and Satish C. Gupta, APS Topical Conference on Shock Compression of Condensed Matter, 2005.**

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**Tensile stress as a function of strain for Mo**

**Tensile stress as a function of strain for Ti, Zr and Hf**
Electrical resistance, TEP and structure variation with pressure for NiSi$_2$.
Investigations on strongly correlated systems

CuIr$_2$S$_4$ with spinel structure is a highly correlated system being investigated for several reasons. It exhibits interplay of structure, transition metal mixed valence (Ir$^{3+}$/Ir$^{4+}$), magnetic ordering, metal-insulator transition, Ir$^{4+}$-Ir$^{4+}$ dimerization, stabilization of an insulating phase at low temperature and high pressure etc. Investigations on CuIr$_2$S$_4$ revealed the existence of a re-entrant metallic phase in it above 30 GPa (Fig. a) and two structural transitions (Fig. b). The manganese based intermetallics, Mn$_3$GaC, with cubic antiperovskite type structure falls in to an intermediate class of materials between the rare earth manganites and the normal metallic alloys. High pressure angle dispersive X-ray diffraction investigations on Mn$_3$GaC up to 35 GPa (Fig. c) aimed at investigating the signatures of the strong interaction between the magnetic and the structural properties of Mn$_3$GaC on the compressibility and its structural stability under pressure did not reveal any anomalies.
High temperature compressibility measurements

Compressibility measurements on solids at high temperature in the piston-cylinder high pressure (PC) apparatus (Fig. a & b), were performed on fused quartz. An apparently first order transition in fused quartz with a volume change of about 20% at 3.6 GPa and 680 °C was observed (Fig. c). The X-ray powder diffraction (XRD) and Raman measurements (Fig. d) on the quenched sample showed the transition to be from a low density amorphous phase to another high density amorphous phase. This work is the first application of PC set up for high temperature compressibility measurement.

High pressure and high temperature studies on negative thermal expansion materials

Negative Thermal Expansion (NTE) is observed in the low-density phases of ionic compounds with MO₄, AO₆, AM₂O₇, A₂M₃O₁₂ and AMO₅ stoichiometry (A & M are octahedral and tetrahedral cations), which have a three-dimensional open network structures with corner sharing polyhedra. NTE materials predisposed to display interesting behavior at high pressure and high temperature. Also such ceramic materials that exhibit NTE are of technological importance because of the ionic conductivity facilitated by cation disorder in them and because of the possibility to tune the thermal expansion of NTE-normal material composites. On our ongoing investigations on these NTE materials we have carried out high pressure and high temperature investigations on Al₂(WO₄)₃, HfMo₂O₈, ZrMo₂O₈ and NbOPO₄ belonging to a new subclass of compounds.

Several structural transitions, a linear pressure volume relation or unusually large variation of bulk modulus over limited pressure region, pressure induced amorphization that fall into two categories (Kinetic hindrance to bond reconstructive transitions and decomposition) and a possibility of synthesis of new phases at high temperature and pressure are the highlights of these investigations.