Report on modelling and materials

EuCARD, Collaboration (EuCARD)

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DELIVERABLE REPORT

REPORT ON MODELLING AND MATERIALS

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Abstract:

The WP8 aims at the design of advanced materials and collimators to allow for higher beam power in state-of-the-art accelerator facilities. Task 8.2 in particular focusses on the research, development, production, characterization and testing of novel materials for advanced thermal management applications primarily devoted to future Phase II Collimators, but having the potential to be applied to a much broader spectrum of applications. A broad variety of materials has been studied, produced and characterized, including metal-diamond composites such as Copper-Diamond, Silver-Diamond, Molybdenum-Diamond as well as Molybdenum-Graphite composites with very promising results. Advanced numerical simulation techniques have been used to study the behaviour of these, as well as more traditional materials under the effect of very intense, highly energetic particle beams. An intensive testing programme is being deployed to verify their behaviour under extreme conditions.

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Delivery Slip

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1. EXECUTIVE SUMMARY

A new family of materials, combining the physical, thermal, electrical and mechanical properties which are required by the extreme working conditions existing in high energy particle accelerators is being developed: Metal Matrix Composites with Diamond or Graphite reinforcements. These materials are to combine the outstanding thermal and physical properties of diamond and graphite with the electrical and mechanical properties of metals.

Materials already produced and characterized include Copper-Diamond, Silver-Diamond, Molybdenum-Diamond and Molybdenum-Graphite.

A comprehensive material testing program, including a first-of-its-kind experiment submitting materials to intense proton beams, is in full swing. These activities are complemented by advanced numerical simulations allowing to study the extreme phenomena which these materials may undergo.

2. INTRODUCTION

The introduction in latest years of new, extremely energetic particle accelerators such as the Large Hadron Collider (LHC) brought about the need for advanced cleaning and protection systems in order to safely increase the beam energy and intensity to unprecedented levels. A key element of the cleaning and protection system is constituted by collimators which are to intercept and absorb the high intensity particle losses unavoidably present in the accelerator and to shield other components from the catastrophic consequences of beam orbit errors.

The collimation system currently installed in the LHC (Phase I) is effectively ensuring the safe operation of the collider in the present operating conditions. However, intrinsic limitations of Phase I collimators may hinder LHC ultimate performances, as to cleaning efficiency, resistive-wall impedance and radiation hardness. Additional advanced collimators (Phase II) are hence to complement the present system to overcome these limitations and comply with the LHC upgrades for the years to come.

One key element to obtain next-generation collimators meeting these requirements lays in the development and use of novel advanced materials for the collimator jaws as no existing metal-based or carbon-based material possesses the combination of physical, thermal, electrical and mechanical properties which are required by the collimator extreme working conditions.

This challenge is part of the task 2 of EuCARD ColMat Work-package (WP8) and is specifically addressed by sub-tasks 3 and 4.

Several families of novel materials have been studied and developed: in this report the activities carried out by partners in task 8.2 (CERN, RHP-Technology, POLITO, RRC-KI, EPFL and GSI) as well as in a collaborating Italian SME (Brevetti Bizz, San Bonifacio, Verona, Italy) for the development, simulation, production, characterization, and testing of each family of these materials are presented.

3. R&D ON NOVEL ADVANCED MATERIALS

This R&D program has been launched having in mind a number of key requirements which must be fulfilled to ensure that next-generation collimators meet their main functions, i.e. *beam cleaning* (i.e. removing from the beam pipes those stray particles which may lead to superconducting magnet quench, i.e. transition from superconducting to normal (resistive) conducting state) and *machine protection*, that is shielding other critical components in case of beam orbit errors with the potential to generate catastrophic consequences. These requirements are essentially low *resistive-wall impedance* so to avoid the RF-induced beam instabilities seriously hampering accelerator performances, high *cleaning efficiency*, implying the ability to rapidly absorb the largest possible number of particles populating the so-called beam halo, high *geometrical stability* to maintain the extreme precision of the collimator jaw during normal operation required by functional specifications and high *structural robustness* in case of accidental scenarios.

It is interesting to note that several of these requirements are common with other advanced thermal management applications, so that the object of this R&D program may have interesting spin-offs on such industries as Aerospace, Medical, Nuclear, Electronics to name a few.

3.1. MATERIAL CLASSIFICATION

In order to classify materials and rank candidates against the criteria defined above, five main figures of merit have been identified. These figures of merit are:

- *Electrical conductivity* **γ**. This parameter has to be maximized in order to limit resistive-wall impedance.
- *Atomic number* **Z**, which provides a rough indication of the material cleaning efficiency. The higher the atomic number, the better the cleaning efficiency.
- *Steady-state Stability Normalized Index* (**SSNI**), defined as $k/(\alpha\rho)$, (k thermal conductivity, α Coefficient of Thermal Expansion, ρ density). SSNI provides an indication of the ability of the material to maintain the geometrical stability of the jaw when submitted to steady-state losses.
- *Transient Thermal Shock Normalized Index* (**TSNI**), defined as $[R(1-\upsilon)\, c_{pv}]/(E\alpha\rho)$ (R mechanical strength, υ Poisson's ratio, c_{pv} volumetric heat capacity, E Young's modulus). TSNI is correlated to the highest absorption rate of impacting particles before the onset of structural damage.
- *Melting Temperature* **T_m** provides an indication of the maximum temperature the material can achieve before being permanently damaged by melting.

On top of these, several other requirements have to be met such as *radiation hardness*, *UHV compatibility*, acceptable brittleness, feasibility of large components on an industrial scale, possibility to machine, braze, join, coat, etc., affordable costs.

Comparison between different materials and identification of suitable candidates is extensively discussed in the conference paper "Advanced Materials for Future Phase II LHC collimators" presented at PAC '09.

The full text is available at https://cdsweb.cern.ch/record/1428516.

3.2. METAL MATRIX COMPOSITES WITH DIAMOND OR GRAPHITE REINFORCEMENTS

Amongst the many possible alternatives, a particular class of Metal Matrix Composites (MMC) seems particularly appealing as it promises to combine the properties of diamond or graphite (high thermal conductivity, low CTE, low density) with those of conducting metals (high electrical conductivity, strength, toughness, etc.): these are MMC with diamond or graphite reinforcements.

The addition of diamond or graphite particles (at varying volume contents) to a metallic matrix (namely copper, silver or molybdenum) can bring the following benefits:

- Reduction of the density (and average atomic number) of the material, permitting a smoother energy distribution and lower thermal gradients.
- Reduction of the Coefficient of Thermal Expansion (CTE).
- Increase the Thermal Conductivity.
- Increase the overall Radiation Hardness of the composite.

The R&D on Metal Diamond materials has been extensively reported in the IPAC 2011 conference paper “Research and Development of Novel Advanced Materials for Next-generation Collimators” (available at https://cdsweb.cern.ch/record/1428445/files/EuCARD-CON-2011-044.pdf).

In the following sections a brief summary of each material family which has been studied is presented.

3.2.1. Copper-Diamond

Copper-Diamond (Cu-CD) has been recently under investigation for thermal management applications in high power electronic devices. The grade we investigated has been developed at RHP-Technology.

The material has been obtained by Rapid Hot Pressing (RHP) of metallic copper, with the addition of small quantities of boron powder, mixed with synthetic diamonds (CD): the RHP technique permits to solid-sinter in a controlled atmosphere the mixture applying a precise pressure and temperature cycle, up to roughly 1000 ºC.

This process permits to achieve very good compaction rates (~95%), without diamond graphitization.

Since no chemical affinity exists between Cu and CD, adhesion must be assured by a third element, in this case Boron (B). B particles form carbides (BC) at the diamond interface and slightly dissolve in Cu, assuring mechanical bridges between the two main phases (Fig. 1).

This interface has however inherent limitations due to the brittleness of Boron Carbides and to the limited contact surface between Cu and CD, which obstructs heat transfer.

In spite of this, Cu-CD represents an interesting candidate for future collimators, although Cu fairly low melting point somehow limits its application for highly energetic accidents.

Cu-CD has been extensively characterized at CERN in collaboration with various partners: RHP Technology (mechanical and thermal properties), EPFL (CTE) and Politecnico di Torino (mechanical properties).

To verify its Radiation Hardness Cu-CD is currently being tested at RRC-KI: the thermo-physical properties of the materials are measured before and after irradiation with proton and carbon-ion beams to assess material degradation to be expected during its life-time inside the LHC machine (fig.2).

Additional irradiation tests have been carried out at GSI with ^{238}U ions, up to a fluence of $1.7 \cdot 10^{14}$ i/cm^2. Crack formation or diamond detachment at the diamond-matrix interfaces were not observed. The evolution of diamond charging behaviour with fluence suggests that charge trapping defects are formed within the diamond by irradiation (fig. 3).

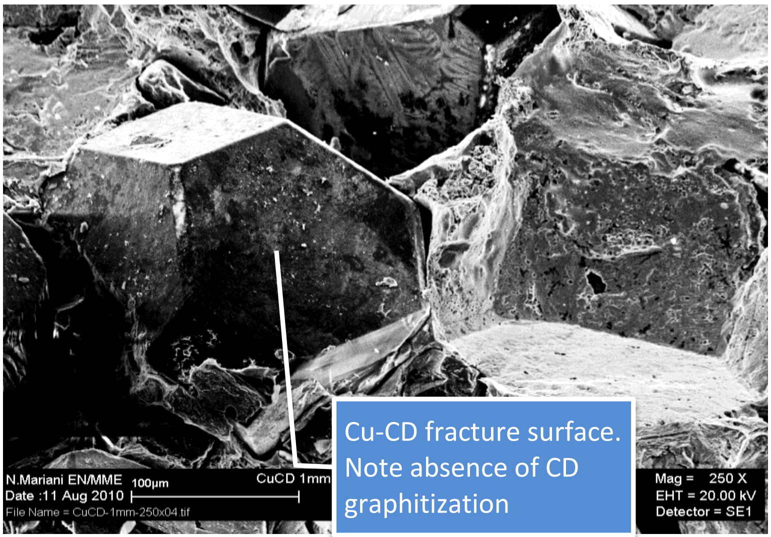

Fig. 1: SEM picture of the fracture surface of Cu-CD. The synthetic diamonds are embedded into Cu matrix which detached during fracture (small BC bridges still attached to diamonds can be observed). CERN.

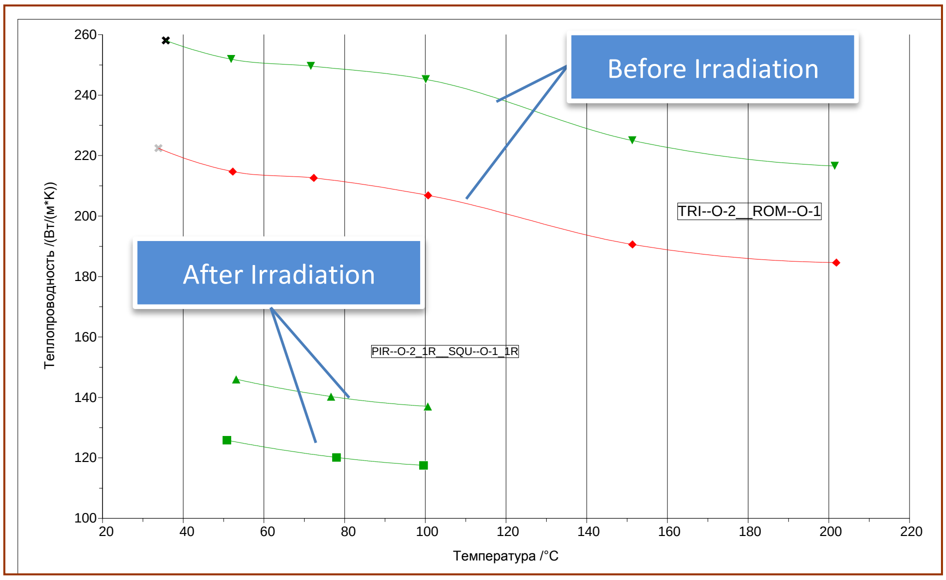

Fig. 2: Thermal conductivity in Cu-CD before and after 30 MeV proton beam irradiation at a dose of 10^{17}p/cm^2. RRC-KI

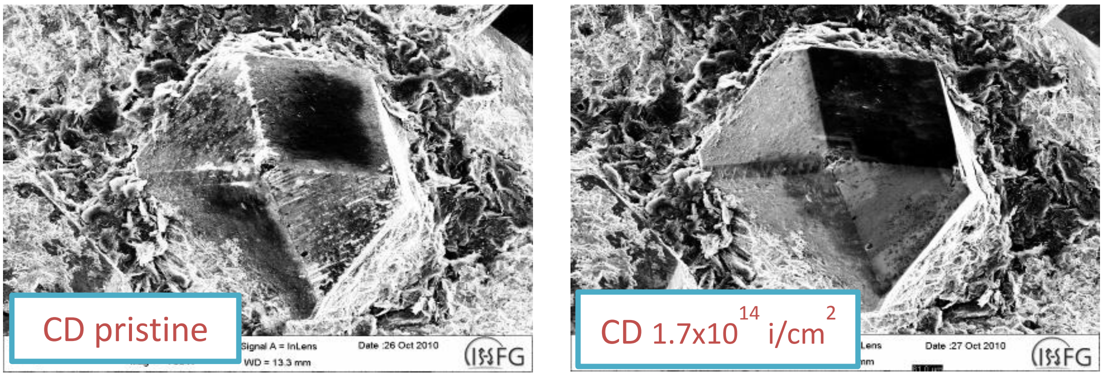

Fig. 3: SEM micrographs of a diamond on the surface of a diamond-copper composite sample, exposed to increasing fluences of ^{238}*U ions, with an Energy of 4.8 MeV/u. GSI*

3.2.2. Silver-Diamond

Silver-Diamond (Ag-CD) has been developed and tested by EPFL using the Liquid Infiltration Technique. Ag-CD (with 3% Si) has shown very good mechanical properties, thanks to the formation of Silicon Carbides on diamond surfaces, as well as excellent thermal properties.

However several drawbacks, such as Ag low melting point (840°C) and non-homogeneities in diamond distribution, complicate its use for Phase II collimators.

3.2.3. Molybdenum-Diamond

CERN is carrying out with a SME (Brevetti Bizz, San Bonifacio, Verona, Italy) an R&D program on Molybdenum-Diamond composites, further enlarging the scope of EuCARD collaboration. The objective of this program is to obtain a composite material combining good thermal and mechanical properties on a broad range of temperatures with a tailored density and acceptable electrical resistivity.

As opposed to Cu, Mo forms stable carbides (Mo_2C) on diamond surface which provide good bonding strength: since Mo_2C has low thermal conductivity and high brittleness, the carbide layer thickness must be kept to a minimum.

Mo-CD is also obtained by RHP technique. Given that the temperature needed to fully sinter Mo (~1700 ºC) is much higher than that of Cu, diamond degradation constitutes the main challenge of the process.

To reduce sintering temperature to an acceptable level (1200-1300°C), while keeping good compaction rates, two different approaches have been tested:

- Liquid Phase Sintering (LPS): a third low-melting phase (typically Cu or Cu-Ag) is added to the mixture to fill in the pores between Mo and CD.
- Assisted Solid-state Sintering (ASS). The addition of small amount of activating elements (typically Ni or Pd) permits to reduce Mo sintering temperature.

Many different combinations of powders, with various liquid phase fillers and diamond coatings have been produced by LPS at Brevetti Bizz and tested at CERN. Samples with dimensions ranging from a few millimetres thickness up to 400x80x20 mm3 (a size comparable to a collimator jaw) (fig. 4) were produced. Values of flexural strength for 13 different compositions are reported in Fig. 5.

Fig. 4: A large Mo-CD sample produced by liquid infiltration. Brevetti Bizz

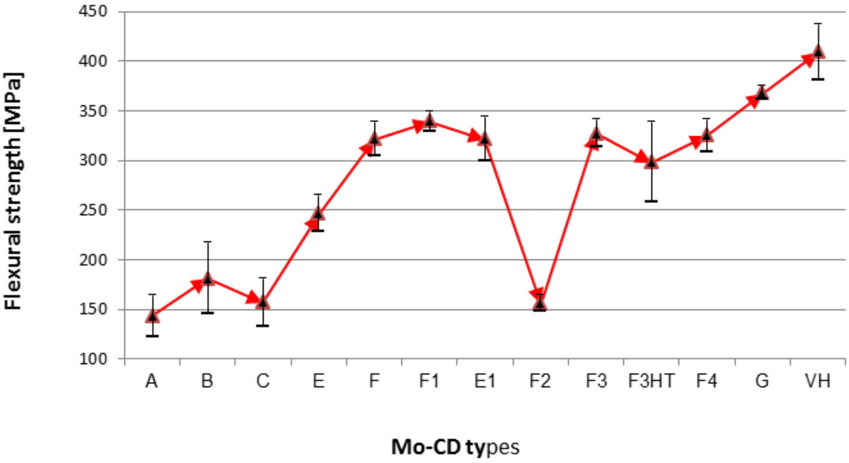

Fig. 5: Flexural Strength of Mo-CD compounds with different liquid phase elements and CD coatings. CERN

The addition of small amounts of activating elements, such as Ni or Pd, brings a significant increase in Mo sintering at relatively low temperatures. Pd was eventually preferred to cheaper Ni as the latter forms a brittle inter-metallic phase with a low melting point. Pd, unlike Ni, is completely soluble in Mo matrix up to 3% in weight, with no secondary phase formation. Mo-Pd compounds were successfully sintered at temperatures as low as 1300 ºC (fig. 6).

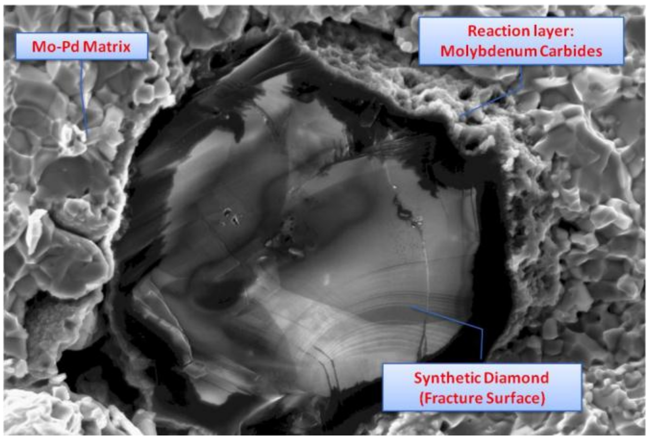

Fig. 6: SEM micrograph of Mo-CD produced by ASS. Note the formation of Mo_2C *at the diamond-matrix interface. CERN*

3.2.4. Molybdenum-Graphite

Studies on Molybdenum-Graphite, a novel composite class with appealing perspective properties, have recently started. The development of this material is being jointly carried out by CERN and Brevetti Bizz. Graphite is a particularly appealing reinforcement because of its peculiar physical properties, namely low CTE, low density, high degradation point and good shock-wave damping. Its thermal conductivity can be very high, close to that of diamond, if specific natural graphite grades or mesophase-pitch-derived synthetic graphites are chosen. The resulting composite is expected to retain good physical and mechanical properties up to very high temperatures (close to 2500 ºC), to possess very low CTE and good thermal conductivity. Additionally, this material is easy to machine and has lower manufacturing costs compared to metal-diamond composites.

A number of samples with various types of reinforcements and varying process parameters have been produced so far (fig. 7).

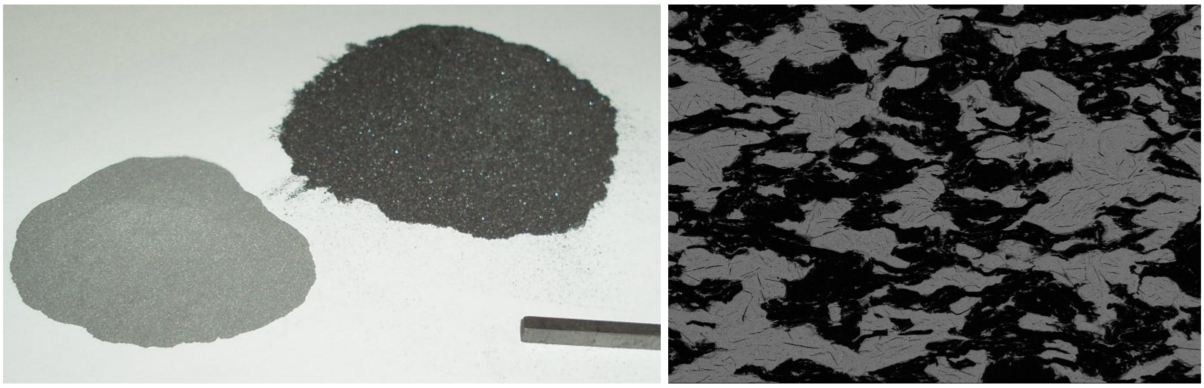

Fig. 7: Mo and Gr powders prior to processing and micrograph of a Mo-Gr sample. Brevetti Bizz, CERN.

To improve the resistive-wall impedance, a cladding with pure molybdenum increasing surface electrical conductivity is also being considered (fig. 8).

The R&D program on Mo-Gr is still in full swing. Significant margins of improvement are expected by optimizing the choice of raw materials, the composition and the process parameters.

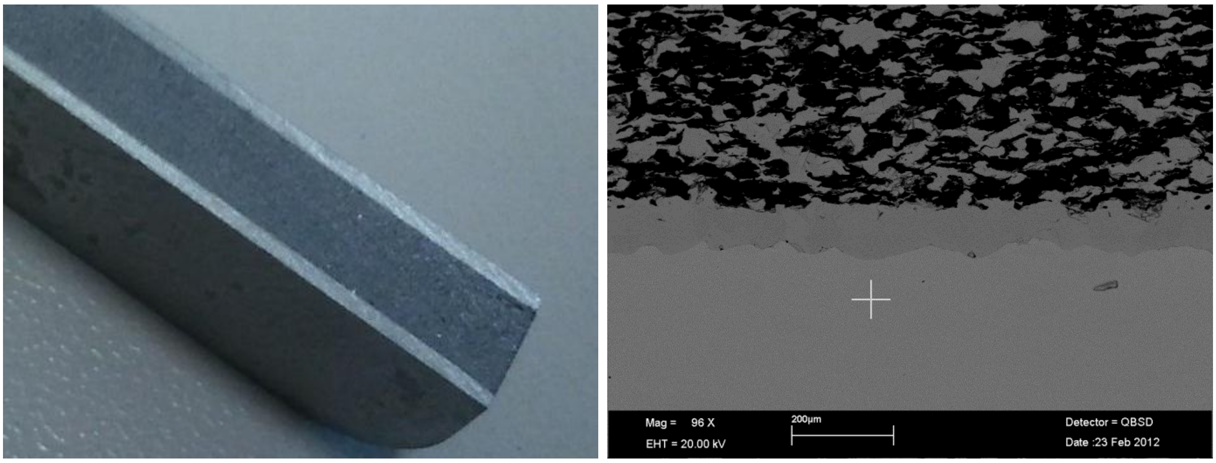

Fig. 8: Picture and micrograph of a Mo-cladded Mo-Gr sample. Brevetti Bizz, CERN

4. NUMERICAL SIMULATIONS

As anticipated above, LHC Collimators, as well as other Beam Intercepting Devices (BID), are inherently exposed to the risk of extended damages induced by energetic particle beams hitting these components. This risk becomes even more severe with the expected increase in beam energies and intensities of the LHC and other future facilities.

Hence, predicting by simulation the consequences of such events, including material phase transitions, extended density changes, shock waves propagation, explosions, material fragment projections etc., becomes a fundamental issue for machine protection: this can be done, to a large extent, by resorting to a new class of wave propagation codes, called Hydrocodes. These are highly non-linear finite element tools, using explicit time integration schemes, developed to study very fast and intense loading on materials and structures.

A considerable experience in computation of structures and materials under extreme conditions using state-of-the-art numerical codes has been gathered at CERN and POLITO, partly in the frame of the EuCARD/ColMat Work Package.

Figure 9 shows the propagation of a shock wave in a Phase I tertiary collimator following the impact of one full LHC particle bunch.

Figure 10 provides an indication of the catastrophic consequences of a very severe accident (8 full LHC bunches) on a tungsten jaw. Hot tungsten fragments are projected with a velocity of almost 1000 m/s and a crater of several millimetres is left on the impacted jaw.

At POLITO additional research is being carried out to couple hydrocodes with *Fluka*, the standard Monte Carlo simulation package for the interaction and transport of particles and nuclei in matter, which provides the energy distribution maps. This original technique allows effectively taking into account the changes of density in the impacted matter occurring during the very short beam impact (fig. 11).

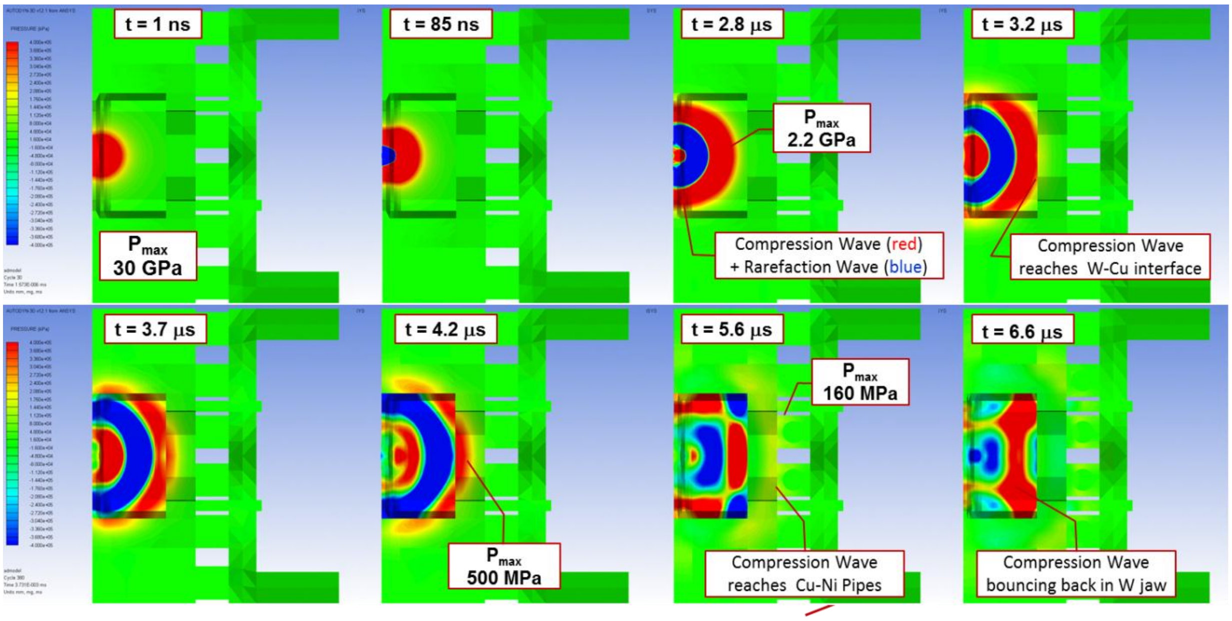

Fig. 9: Sequence of pictures showing the different stages of propagation of a shock wave in a Tertiary Collimator jaw. The component on which the impact occurs and shockwave generates is tungsten made, the surrounding support is copper. In this case damage is mostly confined within the tungsten blocks. CERN

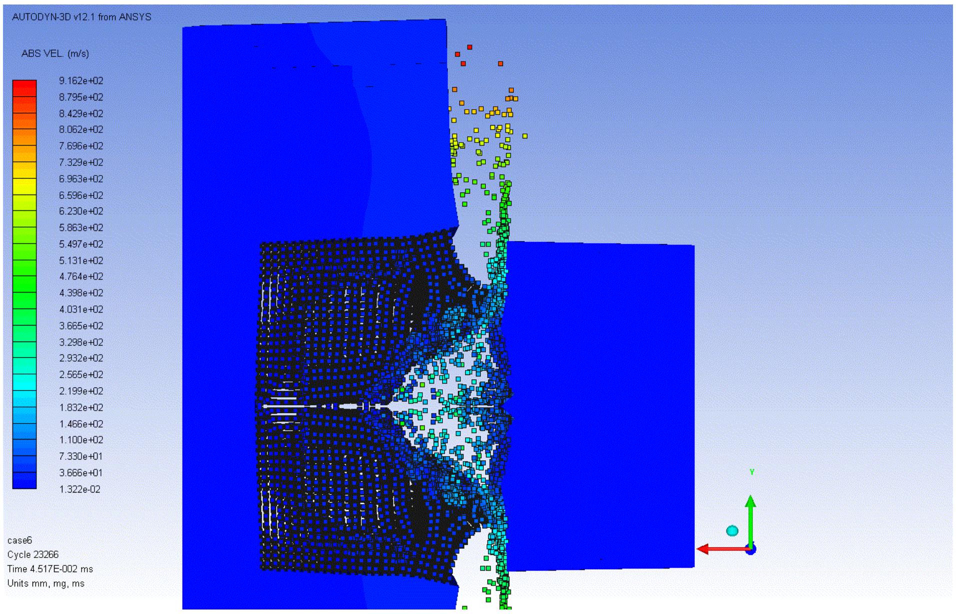

Fig. 10: Projection of high velocity debris out of a tungsten jaw following the impact of 8 LHC bunches, each with 1.3e11 protons at 5 TeV. Opposite jaw is damaged by projected W particles, which are flying with velocities of up to 1000 m/s. CERN

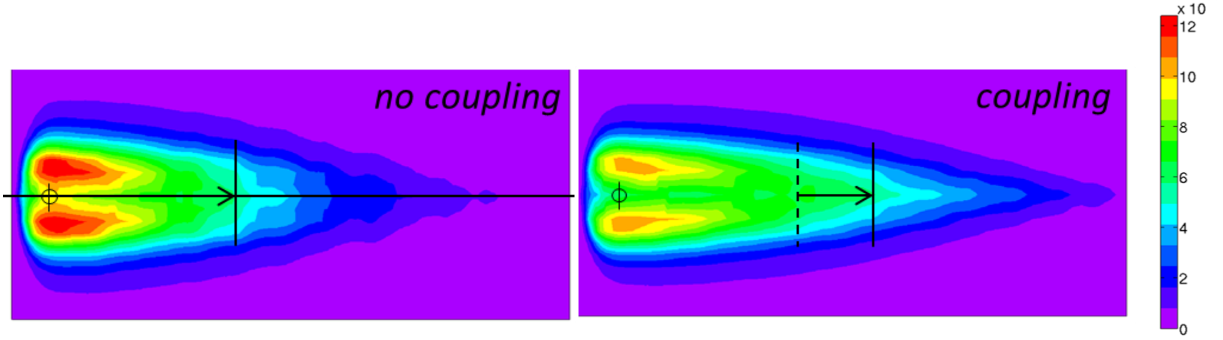

Fig. 11: Differences in density between Fluka/Hydrocode coupled and non-coupled simulations for a copper target impacted by 30 LHC bunches. Note the significant difference in beam penetration (tunnelling effect) between the two cases. Densities are in Pa. POLITO

5. MATERIAL TESTING

A broad range of tests have already been carried out and are planned for the near future in order to fully characterize and qualify novel as well as existing materials under a variety of conditions, environments and operating modes. All task partners have been and are involved at various levels in this effort.

5.1. THERMO-PHYSICAL CHARACTERIZATION

All materials must undergo characterization to assess their thermal and physical properties (density, specific heat, thermal conductivity, CTE, etc.) at room as well as higher temperatures. These tests have been already carried out for the Cu-CD grade produced by RHP-Technology and are expected soon for Mo-CD and Mo-Gr. These characterizations are mainly performed at CERN, either through in-house facilities (fig. 12) or via subcontractors.

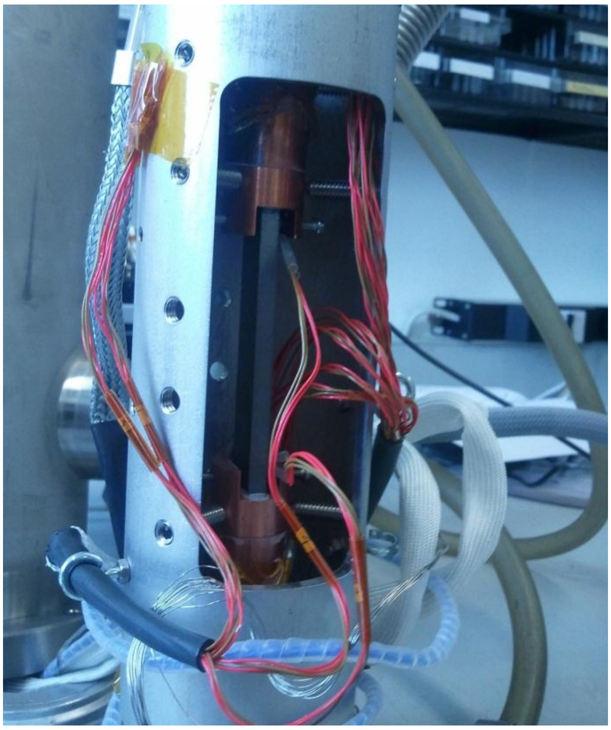

Fig. 12: In-house experimental set-up to measure thermal conductivity in material samples. CERN

5.2. QUASI-STATIC AND DYNAMIC MECHANICAL TESTS

Good mechanical properties are paramount for any engineering application. These properties have been measured for relevant materials both in quasi-static at various temperatures (fig. 13) and in dynamic conditions (fig. 14).

Latter results are particularly important since in the applications of interest loads are very rapidly varying with time and literature data are rather scarce. Measurements have been carried out at CERN and, principally, at POLITO, where sophisticated and optimized equipment to carry out tests at high strain rates is available.

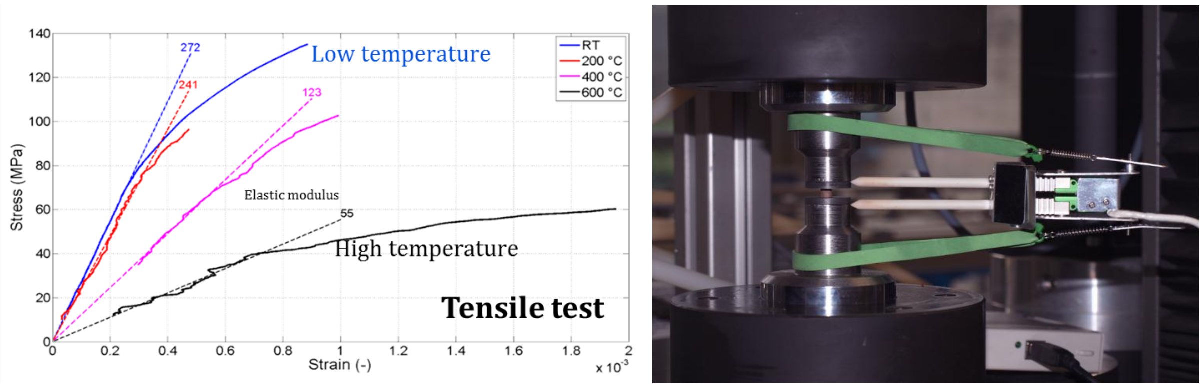

Fig. 13: Quasi-static tensile stress-strain curves for one Mo-CD grade obtained at various temperatures through the experimental apparatus shown on the right. POLITO

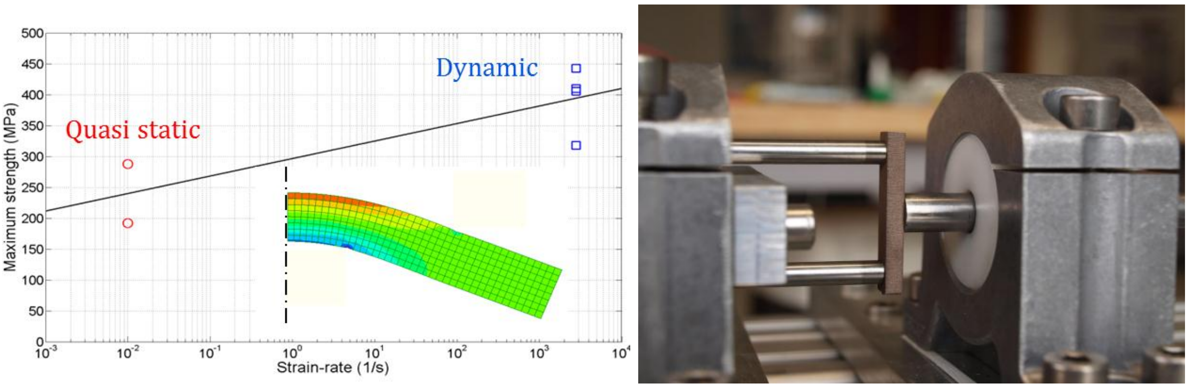

Fig. 14: Maximum bending strength obtained in dynamic conditions, using a new Split Hopkinson Pressure Bar (SHPB) setup, shown on the right. Achieved strain rates are close to 10^4 s^{-1}*. POLITO*

5.3. MATERIAL TESTS IN HIRADMAT

In order for the advanced simulations introduced above to be reliable, the constitutive models of the impacted materials must be accurate over their whole operational range.

Unfortunately, these material models, particularly when reaching extreme conditions as to temperature, pressures and strain rates, are far from being readily available and/or experimentally validated: this is even more the case for the non-conventional compounds and composite materials which are the object of this report.

In order to obtain experimental data upon which building and/or validating reliable constitutive models for relevant materials and benchmarking numerical results (fig. 15), a multi-material sample holder is to be installed in the HiRadMat facility at CERN to test under intense proton beams relevant materials.

The material sample holder is designed and equipped so as to allow an as much as possible complete characterization of each material; additionally, most of the relevant information shall be acquired in real time and made available online.

This challenging experiment, which is to take place by end of 2012, is a first-of-a-kind and, to the best of our knowledge, has never been carried out before. It could also find applications to test materials under very high strain rates and temperatures in other environments (space debris impacts, rocket engines, fast and intense loadings on materials and structures etc.).

The multi-material sample holder is designed in a way to test in the same vessel up to six different materials with two different types of intensity (medium and high) and different material samples (type 1 and type 2) (fig. 16).

Materials to be tested are Inermet 180 (a tungsten grade), Glidcop (copper strengthened by a dispersion of fine alumina), molybdenum, Molybdenum-Diamond (Brevetti Bizz), Copper-Diamond (RHP Technology) and Molybdenum-Graphite (Brevetti Bizz) (fig. 17).

The acquisition system is very complex and designed to acquire information in real-time either with in-situ or remote instrumentation (fig. 18).

The in-situ instrumentation is made up by more than 200 strain gauges and 36 temperature sensors. The sampling frequency of the signals is 5 MHz. Additionally, vacuum sensors and microphones are also installed.

The remote instrumentation is constituted by a Laser Doppler Vibrometer (LDV) measuring radial velocity on the outer surface of type 1 specimens and by a High Speed Camera taking live images of type 2 specimens during and immediately after the beam impact. The capture rate is expected to be in 30000 frames per second range.

This instrumentation is located roughly 40 m away from the experiment in a protected bunker in order to minimize irradiation effects. Images and laser beam are sent to these devices by a series of oriented mirrors.

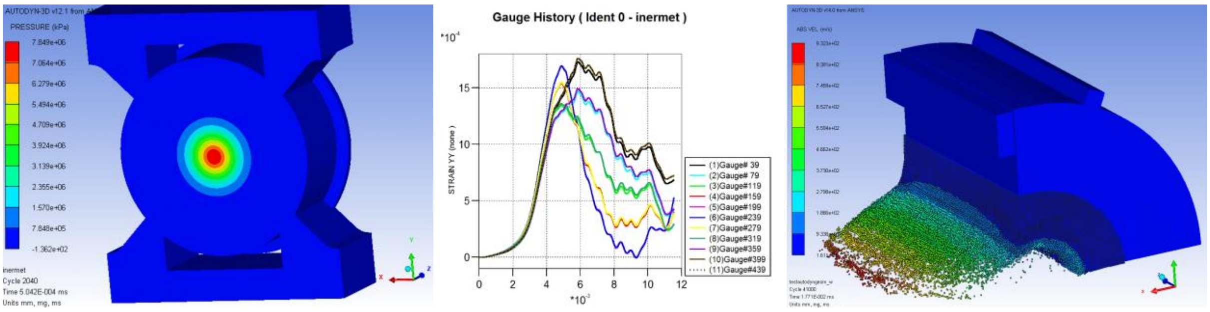

Fig. 15: To the left and centre, pressure after 500 ns (left) and circumferential strains (centre) induced by the impact of 20 HiRadMat bunches (3e12 protons at 440 GeV) on a tungsten cylindrical specimen (type 1). To the right, projection of high velocity particles in a type 2 specimen induced by the impact of 70 bunches. CERN

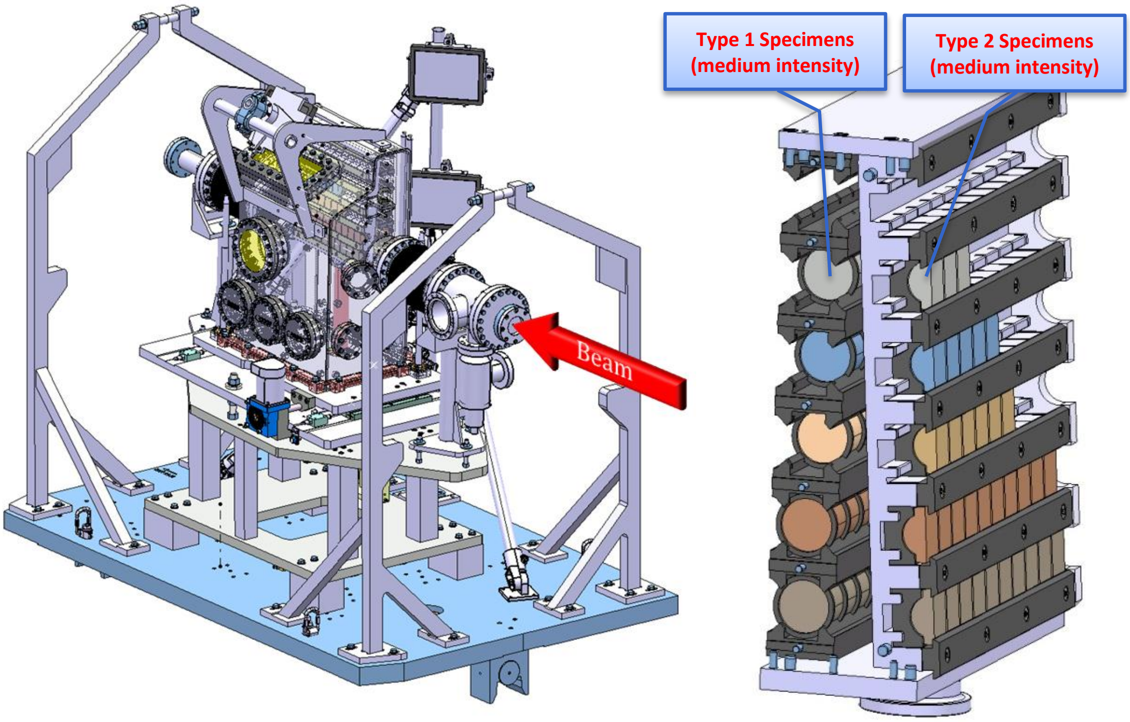

Fig. 16: A 3D model to the multi-material sample holder, now in advanced phase of manufacturing. On the right, the housing, featuring two types of specimens, is shown. CERN

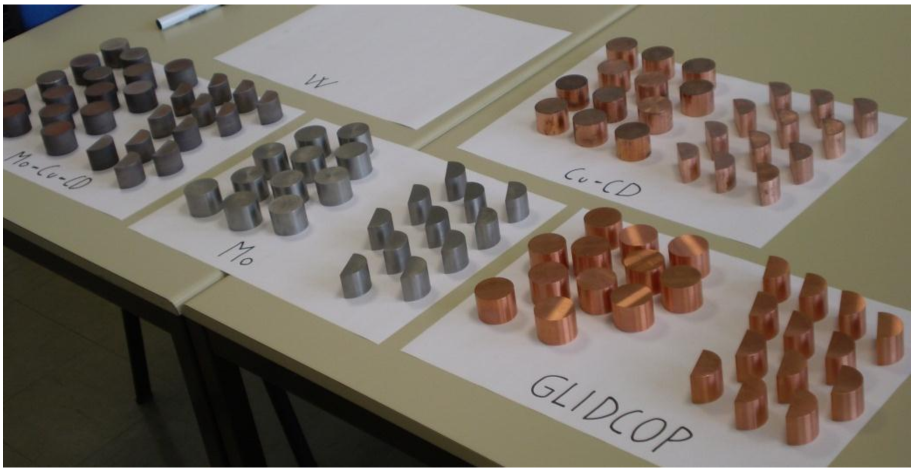

Fig. 17: Type 1 and type 2 specimens of four different materials ready to be mounted in the sample holder. CERN, Brevetti Bizz, RHP Technology

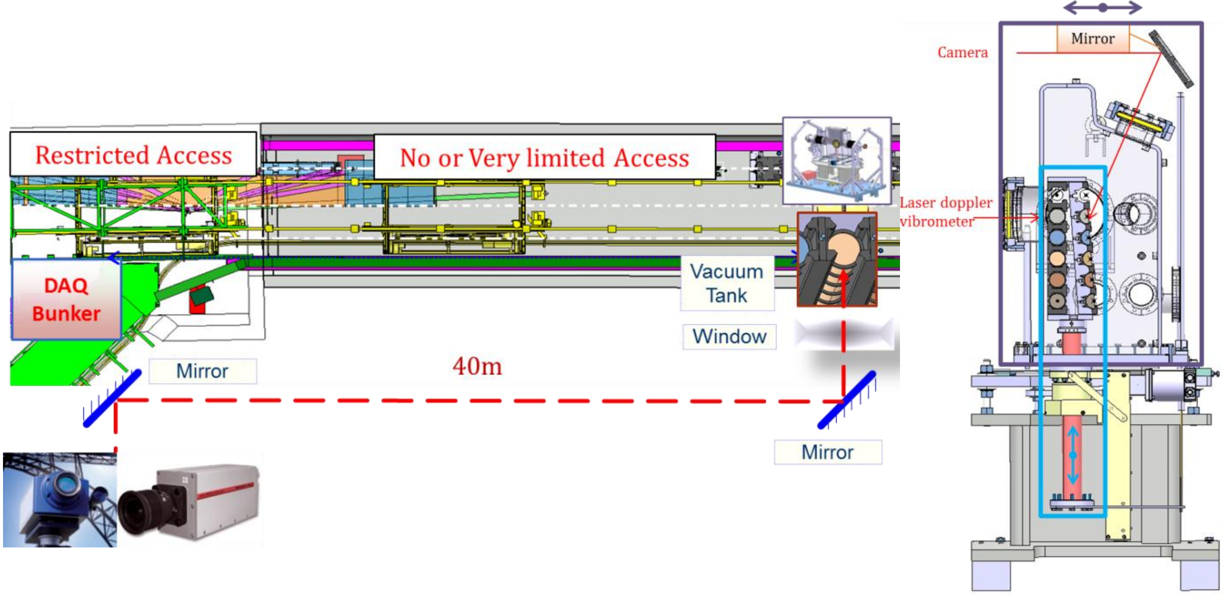

Fig. 18: Layout of the remote acquisition system for the HiRadMat experiment. Note LDV and high speed camera located ~40 m upstream of the test bench.

6. CONCLUSIONS AND FUTURE PLANS

6.1. CONCLUSIONS

Bringing state-of-the-art accelerators such as the LHC beyond today’s performances will likely require a new generation of collimators embarking novel advanced materials.

ColMat Task 8.2 is focusing on the development, simulation and testing of these materials and in the production of prototypes to validate them.

Excellent progress has been made in every aspect of this challenging and far-reaching task with important contributions from many partners.

Metal Matrix Composites with Diamond reinforcement are particularly appealing as they promise to combine diamond and metal properties. Copper-Diamond, Silver-Diamond and Molybdenum-Diamond were studied and successfully produced. The size challenge has been met for Cu-CD and Mo-CD. Their characterization is well advanced and steadily progressing. Radiation hardness assessment is on-going for Cu-CD and to start soon for Mo-CD.

An additional material (Molybdenum-Graphite) is currently under development and promises to further increase the performance reach of Metal Matrix Composites for advanced thermal management applications.

State-of-the-art numerical simulations using complex wave propagation codes (Hydrocodes) have been carried out to study the extreme phenomena induced in matter by the impact of very intense and energetic particle beams.

In order to complete the characterization of these materials, to derive their constitutive models and to benchmark numerical simulations, high intensity tests on material samples of simple geometrical shape, conveniently equipped and monitored are foreseen at CERN. A multi-material sample holder with a challenging DAQ system is currently being prepared for HiRadMat tests in late 2012.

6.2. FUTURE PLANS

The material R&D program is to continue in the coming months, specifically focussing on the improvement of Cu-CD, Mo-CD and Mo-Gr by working on the manufacturing processes and on the identification of enhanced raw materials.

A wealth of data to be analysed, interpreted and turn into constitutive models is expected to come from the HiRadMat experiment.

This R&D program has the potential to go well beyond accelerator physics applications. Materials and techniques being developed may turn out to be very attractive for a number of sectors, including aerospace, electronics, nuclear and medical industries.

7. ANNEX: GLOSSARY

Acronym	**Definition**
Ag-CD	Silver-Diamond Composite
Cu-CD	Copper-Diamond Composite
Mo-CD	Molybdenum-Diamond Composite
Mo-Gr	Molybdenum-Graphite Composite
ASS	Assisted Solid-state Sintering
BID	Beam Intercepting Devices
CTE	Coefficient of Thermal Expansion
DAQ	Digital Acquisition System
LDV	Laser Doppler Vibrometer
LPS	Liquid Phase Sintering
MMC	Metal Matrix Composites
RHP	Rapid Hot Pressing