# University Grant Commission

# Minor Research Project(2007-2012)

**Project Title**

**Study of certain Bulk metalic glasses using pseudopotential theory**


**Final Report by**

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(c) Report of work done:

(i) Brief objective of the project:

The materials proposed for studies in the present project include binary alloys and bulk metallic glasses and other such newly reported materials. These advanced materials will have very important engineering and technological applications, especially in aerodynamic and nuclear industries. They also may exhibit interesting electronic and magnetic and other properties as it is possible to form bulk metallic glasses from many different combinations of these materials. The structure of some of these materials has been studied experimentally. But the theoretical understanding of such materials is still poor. The main objectives of the proposed study are...

(1) To generate form factors using model potential and some recent local field correction functions for computing physical properties of materials using the pseudopotential formalism.
(2) To compute the pair correlation function of these materials and used it to study the collective dynamics and elastic properties of some binary alloys and bulk metallic glasses like $Al_{88}Si_{12}$, $Zr_{48}Nb_8Cu_{12}Be_{24}Fe_8$, $Zr_{61}Cu18.3Ni_{12.8}Al_{7.9}$ and if possible other such materials.
(3) Carry out study of electrical properties of these materials like, electrical resistivity, thermoelectric power and thermal conductivity.

(ii) Work done so far and results achieved and publications, if any, resulting from the work:

The project was started on 1st April, 2013 with initially the literature survey of the subject. Necessary books and computer were purchased and visits were made to the Department of Physics, Sardar Patel University, Vallabh Vidyanagar for literature survey and for initiating collaboration. The work was started after successful installation of software required to carry out the study. All the calculations were carried out using Fortran language. Before running the actual programs, sample runs were carried out and successful results were obtained. This also included reproducing previously reported results using same method and same programming language. This practice gave us confidence about our computational methods.

Two model potentials, one due to Ashcroft's empty core model potential and another developed by us were selected and the form factors were generated in combination with five recent local field correction functions. These form factors are the basic ingredients for carrying out theoretical investigations using pseudopotential formalism. Before selecting the nature of the electron-ion potentials, necessary check for boundary conditions were carried out and also it was confirmed by us that the form factors satisfy the necessary conditions in the long wavelength limit. In a similar way, to include the exchange-correlation effects, we have used five different forms of local field correction functions. It

was ensured that these functions satisfy compressibility sum rule in the long wavelength limit.

The first necessary ingredient to compute the phonon dispersion and related elastic properties is the effective pair potential. In the present work, we have calculated effective pair potential using second order perturbation theory. Another important quantity is the pair correlation function, for which we have adopted the experimental values. Both the properties i.e. pair potential and pair correlation function are used to compute the longitudinal and transverse phono frequencies in the materials of interest using phenomenological approach of Hubbard and Beeby. This approach is simple extension of lattice mechanical theory of solids to non-crystalline materials like metallic glasses and liquids. In literature, there are basically three approaches to compute the phonon dispersion. One due to Hubbard and Beeby, another due to Takeno and Goda and third one due to Bhatia and Singh. Out of these three approaches, we have selected the one by Hubbard and Beeby because it gave better results for non-crystalline materials. In the long wavelength limit, frequencies were linear and hence we have calculated sound velocities and related elastic constants from slope of this graphs.

A binary alloy$Al_{88}Si_{12}$and two bulk metallic glasses $Zr_{48}Nb_8Cu_{12}Be_{24}Fe_8$ and $Zr_{61}Cu18.3Ni_{12.8}Al_{7.9}$ were taken up for study. The collective dynamics and elastic properties viz. Phonon dispersion curves, elastic constants like Young's modulus, shear modulus, bulk modulus, sound velocities' propagation gap in the transverse mode, Debye's temperature and related properties for such new materials were studied using above mentioned methods.

Another aspect which is studied in the present work is structural and electrical transport properties of non-crystalline materials.

It is known that non crystalline materials have different structural properties compared to crystalline one. Hence the study of structure factor and pair correlation function of such materials can give us important information about structural arrangement in such disordered materials. In the present work, we have computed the Ashcroft Langreth partial structure factor of $Ni_{53}Pd_{27}P_{20}$ amorphous alloy. From this information, Bhatia-Thorton partial structure factors are also calculated. Further, total structure factors were also calculated.

This information is used to compute electrical transport properties viz. electrical resistivity, thermoelectric power and thermal conductivity of NiPdP amorphous alloy using Faber-Ziman approach. This approach allows us to compute transport properties of complex systems also. Since the combination include transition metals such as Nickel, the approach of T-matrix involving calculation of finite phase shift would not be appropriate one. On the other hand, the calculation of transport properties using self-consistent method would involve some approximation in the calculations. Thus to avoid such limitations in both the approaches, we have used the Faber-Ziman approach in the present work.

This study generated very good results. The results were presented in the below mentioned National conferences:

(a) Title of the paper :Phonon modes and elastic constant of $Zr_{61}Cu_{18.3}Ni_{12.7}Al_{7.9}$ bulk metalic glass
Authors list : A.M.JOG[1], O.G.MOMIN[2], A.Y.VAHORA[3], Prakruti Chaudhari[4]
National Conference on recent trends in Engineering, Technology and Management (NCEETM)
ISBN NO.: 978-81-923049-9-1

Indus University of Technology and Engineering
Rancharda, Thaltej, Ahmedabad.
31 January- 1 February, 2014.

(b) Title of the paper : Collective dynamics of $Zr_{48}Nb_8Cu_{12}Be_{24}Fe_8$
Authors list : A.M.JOG*, O.G.MOMIN, A.Y.VAHORA[1], B.Y.Thakore[1]
UGC Sponsored one day Seminar on Condensed Matter Physics (CMP-2014) &Short term Training School on X-ray diffraction Techniques.

Department of Physics,
Sardar Patel University,
Vallabh Vidyanagar, Gujarat State.
3rd to 8th March, 2014.

(c) Title of the paper:Electrical transport properties of amorphous $Ni_{53}Pd_{27}Po_{20}$ alloy
Authors list : A.M.JOG[1], O.G.MOMIN[1], Prakruti Chaudhari[2], B.Y.Thakore
UGC sponsored National Conference on Latest Development in Basic and Applied Science

Department of Physics,
M.B. Patel College of Science,
Anand
Dates:

(iii) Has the progress been according to original plan of work:
Yes, the progress has been according to the original plan and results obtained are presented in National Conferences.