# APPENDIX A:

## A.1 Volume-Weighted Average Density Approximation

The density of BMGs could be approximated using the molar-volume weighted average method. In the following derivation, $\rho i$ is the density of each element i, Ai is the atomic weight of each element i, vi is the atomic volume of each element i:

$$\rho i = Ai / vi. \qquad \text{(equation A-1)}$$

If $\chi i$ represents the atomic perfect, vfi is the volume fraction which is equal to:

$$vfi = \chi i\ vi / vtotal, \qquad \text{(equation A-2)}$$

where
$$vtotal = \sum \chi i\ vi. \qquad \text{(equation A-3)}$$

To calculate the density $\rho$ using molar-volume weighted average,

$$\rho = \sum \rho i\ (\chi i\ vi / vtotal\ ). \qquad \text{(equation A-4)}$$

Using equation A-1, the equation A-4 could be rewritten as

$$\rho = \sum \rho i\ \chi i\ (Ai / \rho i) / vtotal, \qquad \text{(equation A-5)}$$

which can be then reduced to:

$$\rho = \sum \chi i\ Ai / vtotal. \qquad \text{(equation A-6)}$$

Substituting equation A-3 into A-6,

$$\rho = (\sum \chi i\ Ai\ )/ (\sum \chi i\ vi), \qquad \text{(equation A-7)}$$

and the final expression becomes

$$\rho = (\sum \chi i\ Ai\ )/ (\sum \chi i\ Ai / \rho i). \qquad \text{(equation A-8)}$$

## A.2 Verification

A literature survey was conducted to record reliable BMG density measurements. Over thirty BMG densities were recorded with various compositions. The actual surveyed densities are plotted against the density calculation using equation A-8. The results for non-P containing BMGs are shown in Figure A-1.

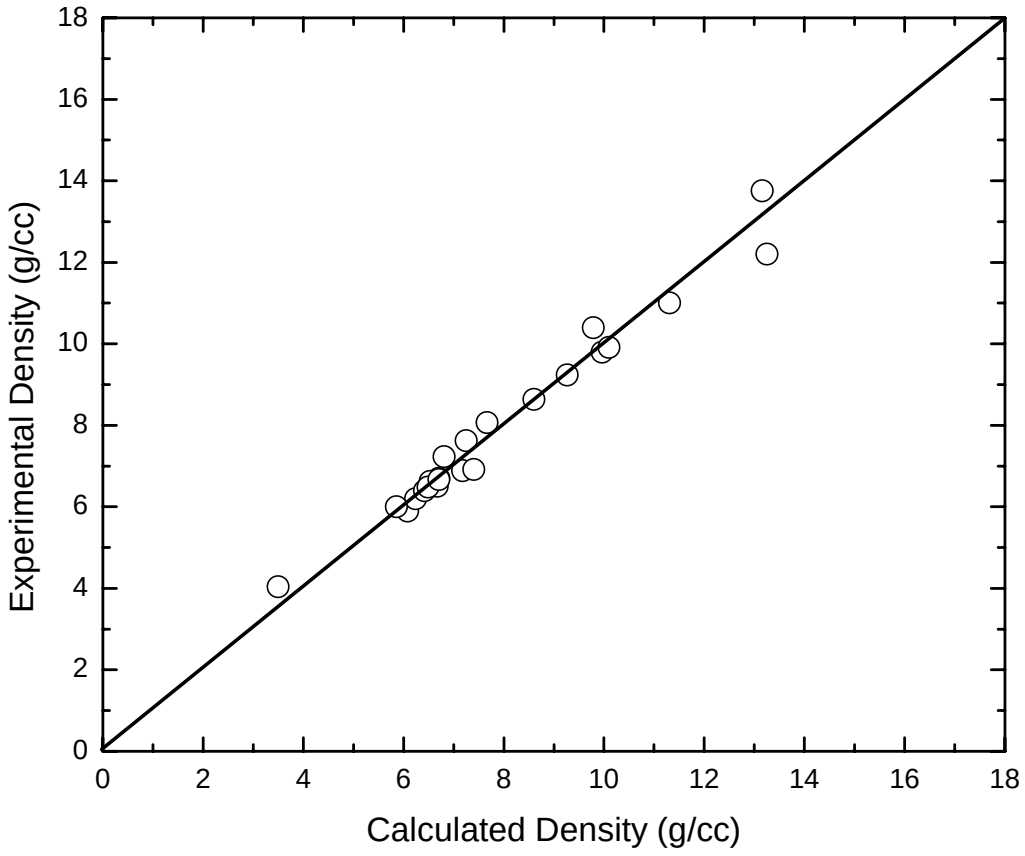


*Figure A-1: Actual BMG alloy densities are plotted against density calculation using molar volume weighted average method. The result shows great agreement between experimental values and calculation.*

The densities for phosphorus-containing BMGs are shown using open hexagons in Figure A-2. Phosphorus is known to "shrink" its atomic radius, especially when the alloy is becoming less covalent and more metallic. The density calculation shows consistent a trend for underestimating P-containing alloys, as shown in Figure A-2.

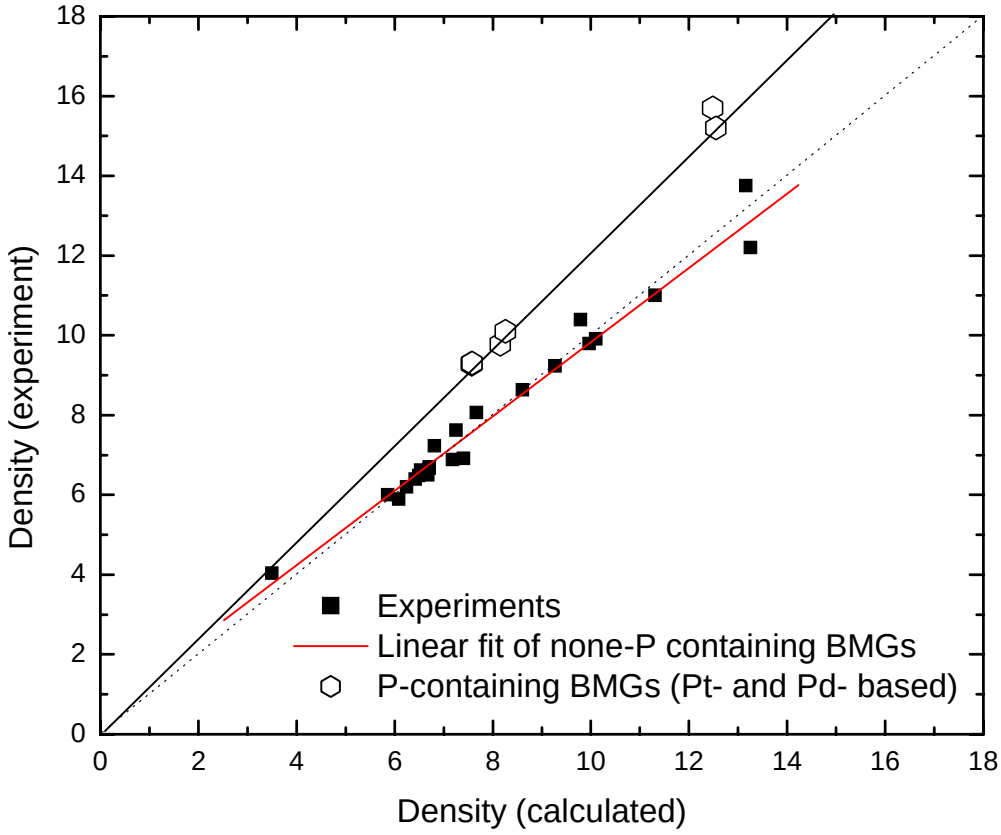


*Figure A-2: Actual BMG alloy densities are plotted against density calculation using molar volume weighted average method. Phosphorus containing alloys (which are Pt- and Pd- alloys) are represented by open hexagons.*