MATERIALS OPTIMIZATION FOR HCCI ENGINES THROUGH COMPUTATIONAL DESIGN

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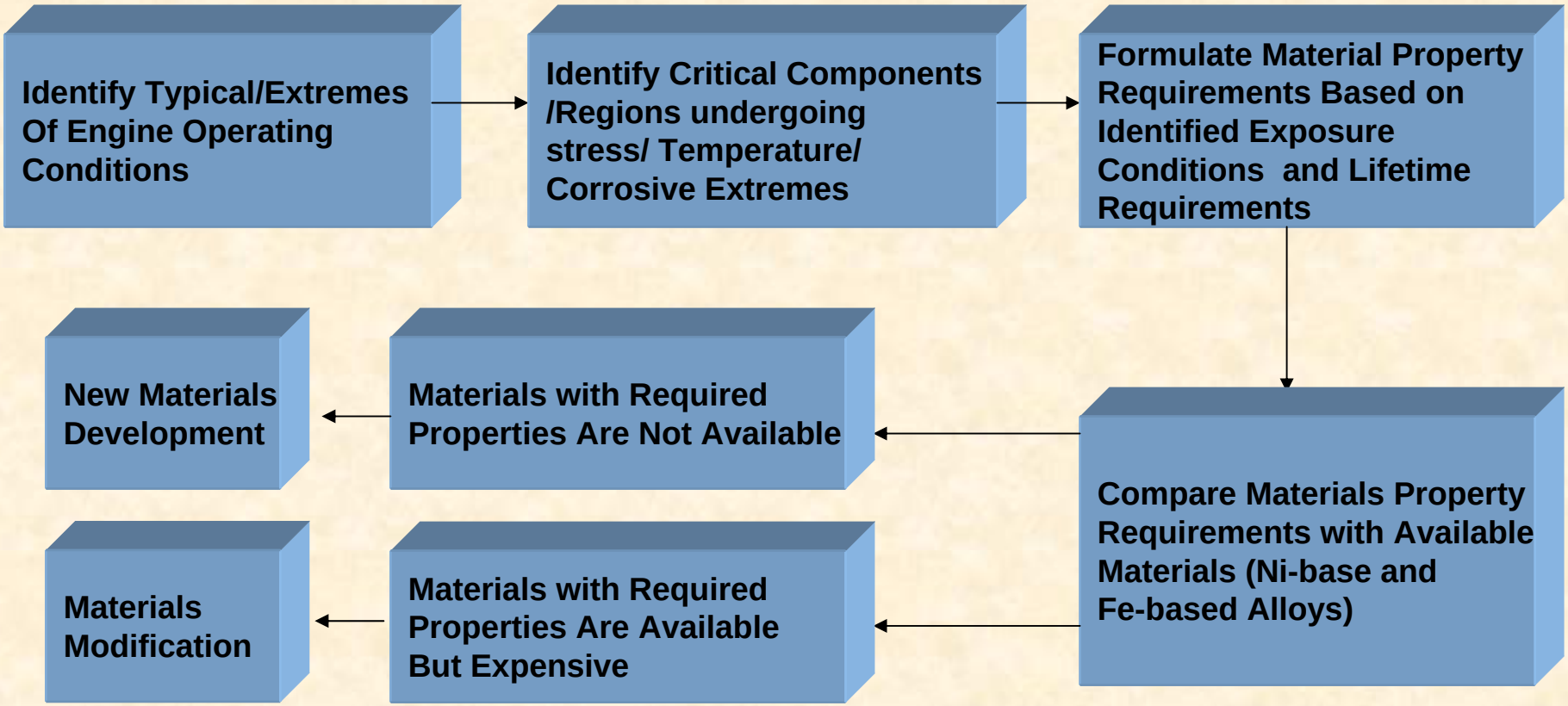
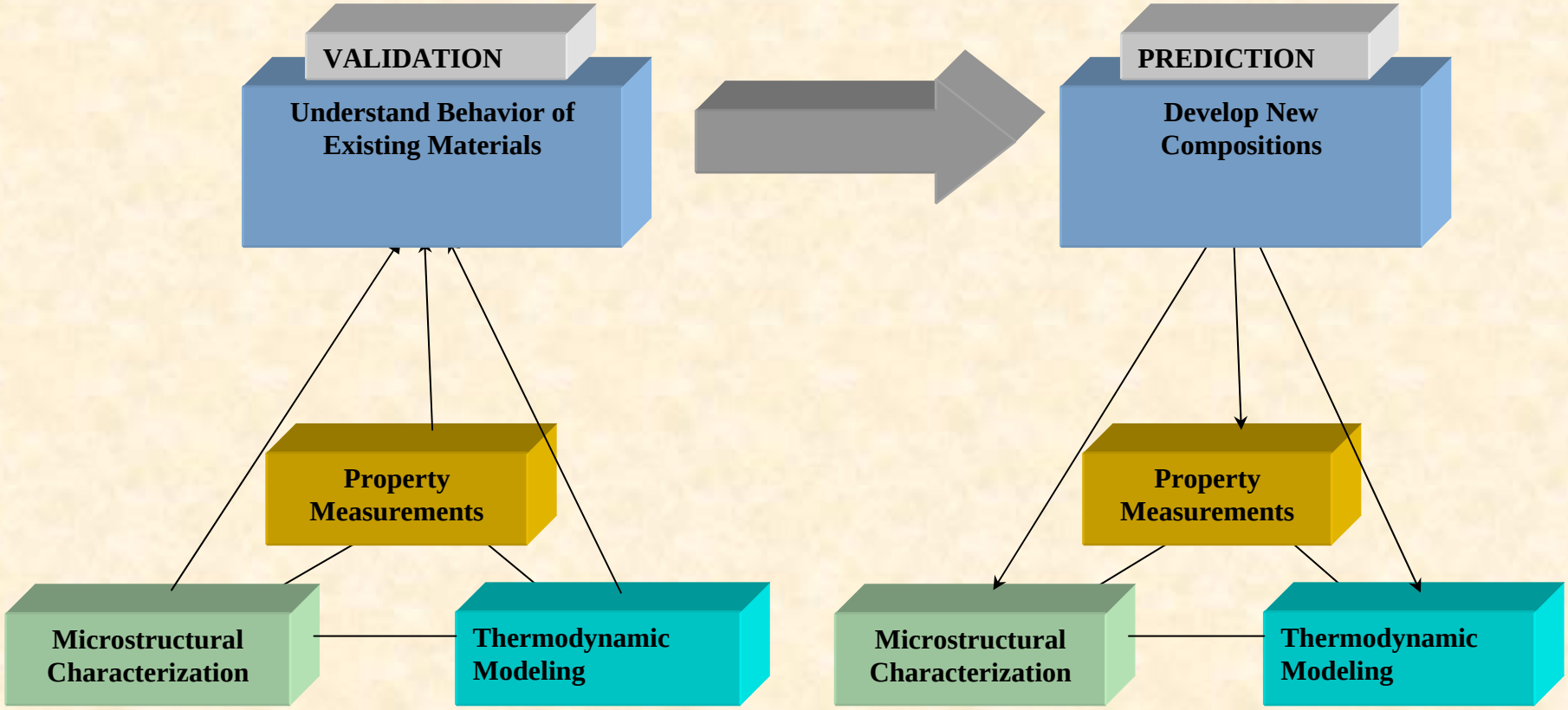
Is there a Need For Materials Development for Advanced Engines?

- **Advanced engines may operate at higher temperatures and/or pressures compared to existing engines**
- **May need new materials with improved higher temperature performance**
  - **New materials may be enhancement of existing materials with small compositional changes, or**
  - **May be completely new for this application**
- **Significant cost (and time) associated with developing new materials through purely trial-and-error experimental techniques**
- **Need to accelerate this process through a well-defined path to developing new materials**

Typical Flow Chart for the Accelerated Development of Materials



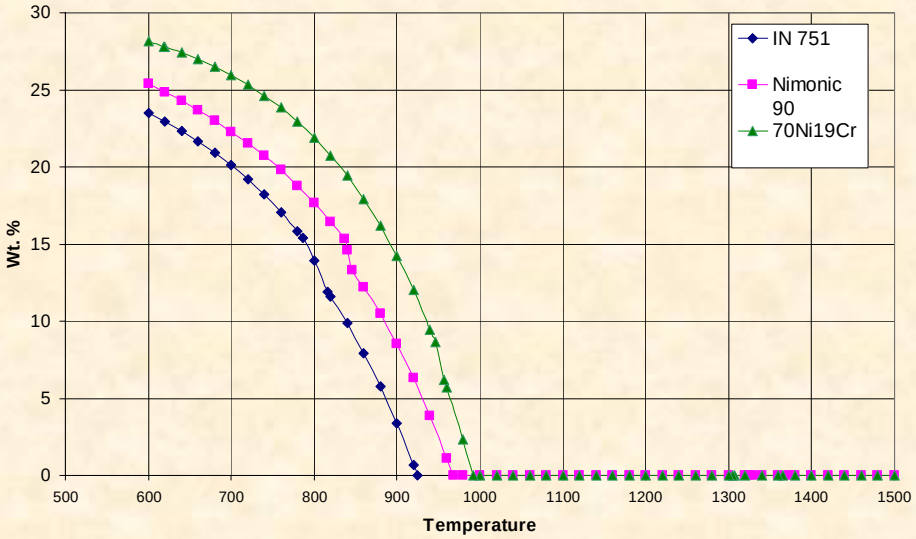
Overall Technical Approach

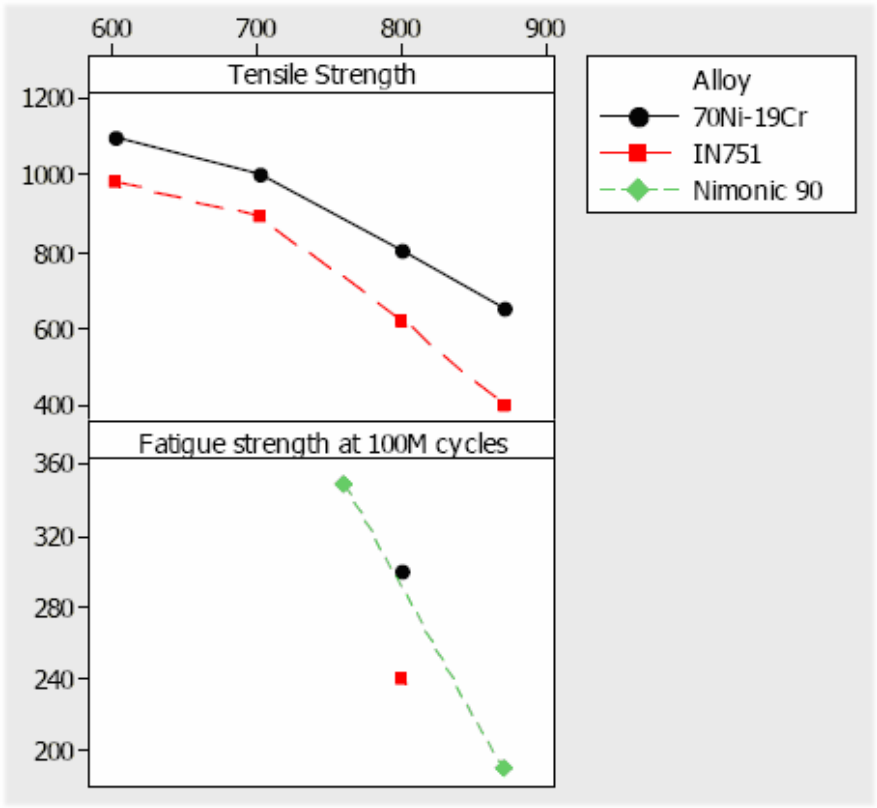


Focus of Current HCCI Project

- **Design/identification of advanced materials for exhaust valves was identified as an area of interest**
- **Property of significant interest is high temperature fatigue life (750°C to 850°C)**
- **A few target alloys were down-selected**
  - **IN 751**
  - **Nimonic 90**
  - **70Ni-19Cr**
- **Correlation was attempted between mechanical properties and calculated microstructure**

Thermodynamic Modeling of γ' Phase Fraction and Relationship to Mechanical Properties





Knowledge of γ' Volume Fraction is Necessary but not Sufficient

Progress in Correlating Mechanical Property Data with Composition

- **Issues:**
  - **Lack of reliable data on relationship between high temperature fatigue property and specific alloy composition (only nominal composition or composition range information available)**
  - **Lack of detailed microstructural information to enable development of quantitative correlations between microstructure and property**
  - **Kinetic factors are important**
- **On-going/ Future work**
  - **Mechanical property measurement in alloys with well-defined compositions and microstructure**
  - **Microstructure evaluation and correlation with thermodynamic and kinetic modeling**