CHAPTER VI

CONCLUSIONS

6.1 Summary and conclusions

Our main objective was to include the photon field variation in the photoemission calculation. For actual photoemission calculation, one has to calculate the initial and final sates involved in the matrix element (equation 1.1). The free electron potential model with a step potential functions at the surface was used for calculating the wavefunctions. We have used the simple model given by Bagchi & Kar[33] for the photon field at the surface. This model was employed for the case of aluminium for which the photocurrent from the Fermi level was calculated. The matrix element has been evaluated numerically and our results[38] show a reasonable agreement with experiment[20] and previous calculations[22] with other models for the fields. The results were analyzed for various values of the surface region, the decay length due to inelastic collisions etc., and the behaviour of the photocurrent as a function of photon energy was studied. It was observed that although some features of the calculated photocurrent (e.g., the minimum at the plasmon frequency were not sensitive to the length of the surface region, some other features (e.g., the ratio of the peak heights below and above the plasmon frequency) were sensitive to it. Also it appeared that even for a reasonable choice of the length 'a' of the surface region - the peak below the plasmon frequency was much sharper in our calculation than was obtained experimentally. However, for the proper description of the metal one has to include the crystal potential to get the correct band structure and the density of states. We have next considered the case of replacing the free electron initial state by a state where the crystal potential, in muffin-tin form was included. Normal photocurrent for the aluminium (100) face was again computed[41] and

compared with the experimental data as well as the free electron calculation. It seems that the results look better when the surface region for the photon field was taken to be the same as the first layer as compared to first two layers. this probably is an artifact of the model rather than the real situation.

We have also derived the formalism for considering both initial and final states in the presence of crystal potential in muffin-tin form. The calculation of these states are along the lines given by Pendry[28], but the presence of the spatially varying field makes the computation of the matrix much more involved. Numerical results for this calculation are not yet available. It may be mentioned here that, although we have used a particular form of the spatially varying photon field, any form of the photon field which is a function of z can be used in our photocurrent calculation. Also, our formalism to calculate photoemission cross-section is applicable to elements whose band structure can be computed with muffin-tin potential.

We have calculated[52] the self-consistent local dipole field near the surface of dipolar lattices. Here we have considered three different structures - the simple hexagonal, hexagonal close-packed and diamond. For the computation of the self-consistent local field we consider a slab geometry of a finite number of lattice planes parallel to the surface. We have carried out the dipole summation plane by plane parallel to the surface of the slab from any chosen origin inside the slab. We also calculated the dipole moment for each plane for three different lattice structures and compared with the experimental data. We have studied diamond structure in more detail and obtained some interesting features. In case of diamond, for some values of the volume polarizability the dipole moments show a oscillatory behaviour -

although the oscillations in the dipolar fields are small. The fields in the surface layer are somewhat different from the bulk local field except for the simple hexagonal structure. We have seen a close resemblance between hexagonal close-packed structure and the fcc structure in the calculation of dipole fields.

6.2 List of Publications

a)Journals:

i] Photoemission Calculation with a Simple Model for the Photon Field: Application to Aluminium ; P Das, R K Thapa & N Kar, *Mod. Phys. Lett.* B, 5 65 (1991) (copy enclosed)

ii] Dipolar Fields Near the Surface for Crystals with Simple Hexagonal, Hexagonal Close Packed and Diamond Structure ; P Das and N Kar; *Mod. Phys Lett.* B, 6 1263 (1992) (copy enclosed)

iii]Electromagnetic fields near metal surfaces; R K Thapa, P Das, N Kar & R A Lal; *Bull. Mat. Sci.* **16** 29 (1993)

iv] Photoemission Calculation with Kronig-Penney Model; R.K. Thapa, P. Das & N. Kar, Mod. Phys. Lett. B,8 361 (1994) (copy enclosed)

v] Photoemission Calculation Including Both Band Structure Effects and Photon Field Variation; P.Das and N.Kar; Phys. stat. sol. (b) **187**, 551 (1995) (copy enclosed)

b) Proceedings of Symposium/Seminar

i] Local field near the surface of a lattice with diamond structure: P Das & N Kar, *DAE Solid State Physics Symposium* 34C, 392 (1991)

ii] Photoemission calculation including both band structure effects and photon field variation ; P Das & N Kar, *DAE Solid State Physics Symposium* 34C, 393 (1991)

iii] Photoemission calculation with free electron wavefunctions and 'local' model of surface ; R K Thapa, P Das & N Kar, *DAE Solid State Physics Symposium* 32C, 396(1989)

iv] Frequency-dependent photoemission from aluminium using a simple dielectric model ; R K Thapa, P Das & N Kar, (Presented at the Young Physicists' Colloquium 1990), *Physics Teacher*, **33** 21 (1991)

v] Photoemission from the surface of silicon using a simple local dielectric model ; R K Thapa, P Das & N Kar, *Proceedings of Conference on Physics and Technology of Semiconductor Devices and Integrated Circuits*, 5-7 Feb'1992, page-318-20.

vi] Photoemission Calculation Including Photon Field variation In The Surface Region; P.Das, DAE SSP symposium'93, **36C** 46 (1993)

vii] Photoemission Calculation from the Fermi Level of Aluminium; P.Das, R.K.Thapa & N.Kar, DAE SSP symposium'93, **36C** 485 (1993)

6.3 References

1. H Hertz, *Ann. Physik* 31 983 (1887)

2. A Einstein, *Ann. Physik* 17 132 (1905)

3. D R Penn, *Phys. Rev. Lett.* 28 1041 (1972)

4. D D Koelling, G Arbman, *J Phys.* F5 2041 (1975)

5. P M Haltham *et al*, *J Phys* F7 635 (1977)

6. H L Skriver, *Phys. Rev.* B14 5187 (1976) & B15 1894 (1977)

7. J P Jan *et al*, *J Phys.* F7 957 (1977)

8. R V Kasowski, *Phys. Rev.* B8 1378 (1973), *Phys. Rev. Lett.* 33 83 (1974), *Solid. St. Commun.* 14 103 (1974) & 17 179 (1975)

9. O Jepsen, *Phys. Rev.* B12 2988 (1975)

10. O Jepsen *et al*, *Phys. Rev.* B12 3084 (1975)

11. G D Mahan, *Phys. Rev.* B2 4332 (1970), *Phys. Rev. Lett.* 24

12. I Adawi, *Phys. Rev.* 134 A788 (1964)

13. N W Ashcroft & W L Schaich, *Solid St. Commun.* 8 1959 (1970), *Phys. Rev.* B3 2452 19 (1971)

14. J G Endriz, *Phys. Rev.* B7 3464 (1973)

15. K Mitchell, *Proc. R. Soc.* A 146 442 (1934), *Proc Camb. Philos. Soc.* 31 416 (1935)

16. R E B Makinson, *Proc. R. Soc.* A 162 367 (1937)

17. K L Kliewer, *Phys. Rev. Lett.* 33 900 (1974) *Phys. Rev.* B14 1412 (1976)

18. T Maniv & H Metiu, *Phys. Rev.* 22 4731 (1980),

19. P J Feibelman, *Phys. Rev.* B12 1319 (1975), *Phys Rev. Lett.* 34 1092 (1975)

20. H J Levinson, E W Plummer & P J Feibelman, *Phys. Rev. Lett.* 43 953 (1979); *J. Vac. Sci. Technol* 17 216 (1980)

21. K Kempa & F Forstman, *Surf Sci.* **129** 516 (1983); K Kempa & R R Gerhardts, *Sol. State Comm.* 53 579 (1985)

22. N Barberan & J E Inglesfield, *J. Phys.* **C 14** 3114 (1981)

23. B C Meyers & T E Feuchtwang, *Phys. Rev.B* **27** 2030 (1983)

24. J T Lee & W L Schaich, *Phys. Rev. B* **38** 3747 (1988)

25. N D Lang & W Kohn, *Phys. Rev.* B1 4555 (1970)

26. G Mukhopadhay & S Lundsqvist, *Physica Scripta* **17** 69 (1978)

27. A Liebsch, *Phys. Rev. Lett.* **32** 1203 (1974),*Phys. Rev.* B13 544 (1976), *Solid St. Commun.* **19** 1193 (1976)

28. J B Pendry, *Surf. Sci.* **57** 679 (1976), *Photoemission and the Electronic Properties of Surfaces*, eds, B Feurbacher, Fitton and R F Willis (Wiley, NY, 1978)

29. J B Pendry & J F L Hopkinson, *J. Phys. F Met. Phys.* **8** 1009 (1978)

30. N Kar, *J. of Phys.* **C 14** 2185 (1981)

31. A Ishii & T Aisaka, *Surf. Sci.* **242** 250 (1991)

32. H J Levinson, F Greuter & E W Plummer, *Phys. Rev.* **B 27** 727 (1983)

33. A Bagchi & N.Kar, *Phys. Rev.* **B 18** 5248 (1978)

34. R K Thapa, P Das *et al*, Bull. Mat. Sci **16** 29 (1993)

35. J Weaver, *Hand Book of Chemistry and Physics of Solids* (CRC Press Boca Raton, Ohio, 1978)E-377

36. J B Pendry, *Low Energy Electron Diffraction* (Academic Press, 1974)

37. N W Ashcroft & N D Mermin, *Solid State Physics* (Holt, Reinhart and Winston, NY, 1976)p- 38

38. P Das, R K Thapa & N Kar, Mod. Phys. Lett. **B 5** 65 (1991)

39. R.K.Thapa & N.Kar; *Phys. Rev.* B 51 1995 (to be published)

40. R.K.Thapa, P.Das & N.Kar, *Mod. Phys. Lett.* **B 8** 361 (1994); R.K.Thapa; *Phys. Stat. Sol (b)* 179, 621 (1993)

41. P.Das and N.Kar, *Phys. Stat. Sol.* (b) **187**, 551 (1995)

42. I S Gradshteyn & I M Ryzhik, *Table of Integrals* (Academic Press, 1980)

43. F L Hopkinson, J B Pendry & D J Titterington, *Comput. Phys. Commun.* **19** 69 (1980)

44. L F Matheiss, *Phys. Rev.* **139** A 1893 (1965)

45. J Hermanson, *Solid St. Commun.* **22** 9 (1977)

46. M Born and E Wolf, *Principles of Optics*, section 2.3, Pergamon press, New York (1970)

47. B R A Nijboer & F W de Wette, *Physica* **24**, 422(1958)

48. N Kar and A Bagchi, *Solid St. Commun.* **33**,645(1980)

49. R Shuttleworth, *Proc. Phys. Soc.* (London) **A62**, 67 (1949)

50. G D Mahan, *J. Chem. Phys.* **43**, 1569 (1965)

51. F W De Wette, *Phys. Rev.* **123**, **103** (1961)

52. P Das & N Kar, *Mod. Phys. Lett.* **B 6** 1263 (1992)

53. P Das & N Kar, Mod. Phys. Lett. **B**, (accepted for publication)